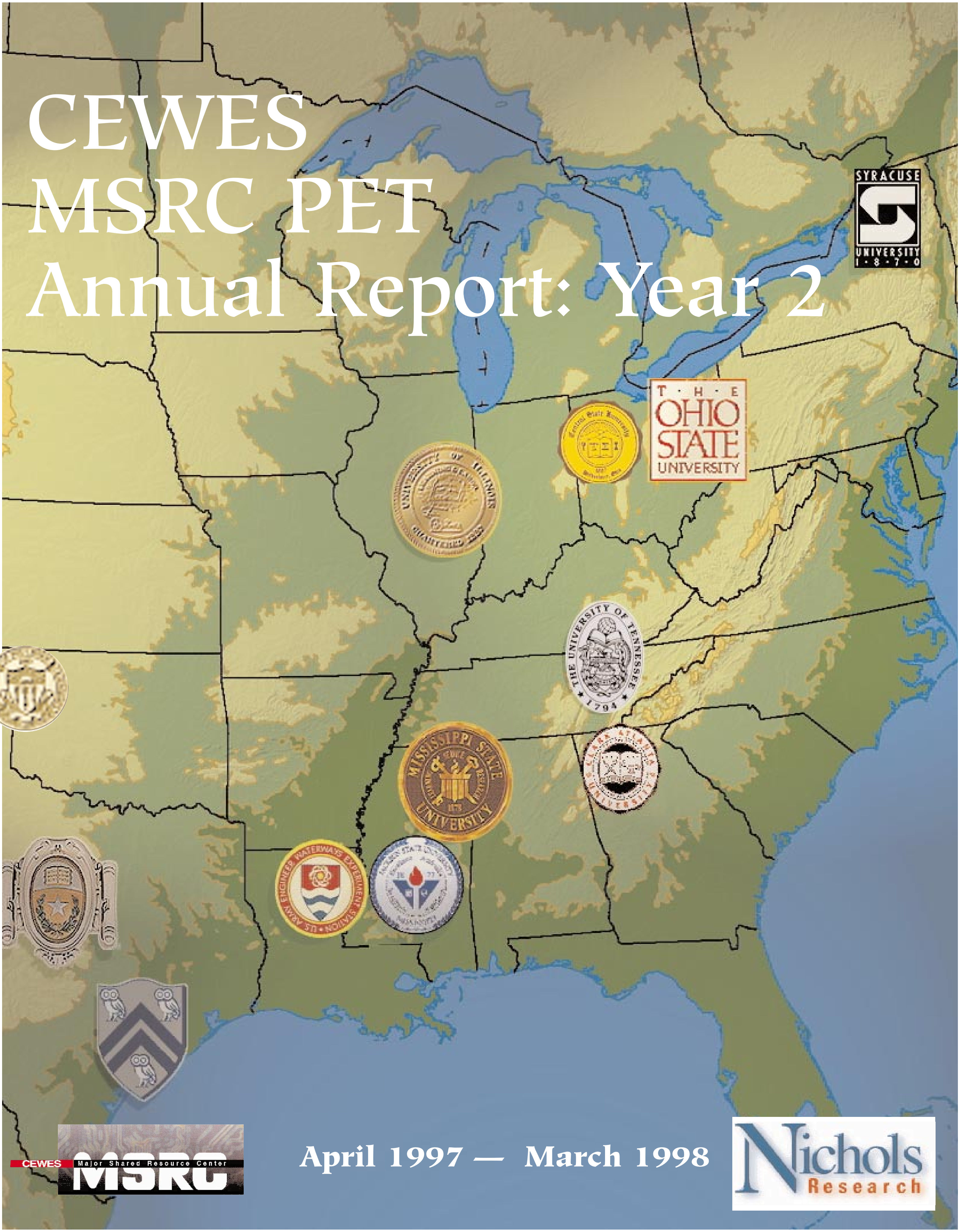
CEWES MSRC PET Annual Report: Year 2



April 1997 — March 1998

EXECUTIVE SUMMARY

The true deliverable of the CEWES MSRC PET effort is the raised level of CEWES MSRC user capability and programming environment in the CEWES MSRC – to a level not surpassed by academic, industry, or other government HPC centers. The CEWES MSRC PET team addresses this charge by providing core support to CEWES MSRC users, performing specific focused efforts designed to introduce new tools and computational technology into the CEWES MSRC, conducting training courses and workshops for CEWES MSRC users, and operating an HBCU/MI enhancement program.

The Programming Environment & Training (PET) component of the DoD HPC MSRCs is a bold and innovative university/industry/government effort to provide the essential user support and mode of capability enhancement that is necessary for the MSRCs to reach a level comparable to that in the foremost university, industry, and other Government agency HPC centers – and to address the wide variety of research and development demands arising from the science and technology programs supporting DoD's weapons development and warfighting support systems. The purpose of the PET component of the MSRCs is to enhance the entire programming environment for the MSRC users through training and support for software enhancement, addressing both near–term improvements and long–term expansions, thus enabling use of the MSRC computing resources to fullest capacity and extending the range of applicability of HPC to DoD technical problems.

The PET effort is unprecedented in its concept and vision, in its management for long–term achievement, in its strong university commitment, in its approach through unique university/DoD collaboration, in its understanding and relationship between university researchers and MSRC users – and in its challenge to be faced in the interest of DoD by the universities and companies involved, the MSRC users, and the program management. The PET component of the MSRC program is thus a true intellectual enterprise which breaks new ground in collaborative effort between DoD and academia in order to establish a two–way conduit of information and expertise enhancing the capability of the MSRC user and bringing demands of DoD HPC to bear early–on in programming environment developments in progress in the universities.

The CEWES MSRC PET effort is administered by the integrator, Nichols Research Corporation (NRC), for the CEWES MSRC as a part of the contract for the CEWES MSRC. Dr Dick Pritchard of Nichols Research is the PET Director. Dr Joe Thompson of Mississippi State University is CEWES MSRC PET academic team leader. Dr Wayne Mastin of Nichols, and a professor–emeritus of Mississippi State, is the on–site PET team leader. Dr Willie Brown of Jackson State University is the HBCU/MI leader. Dr Louis Turcotte of the CEWES MSRC excercises oversight of the CEWES MSRC PET effort for the government.

The fundamental mode of operation for PET at the CEWES MSRC is a direct and continual connection between the CEWES MSRC users and the CEWES MSRC PET team universities in support of the five Computational Technology Areas (CTAs) supported at the CEWES MSRC and three related technical infrastructure areas. This is accomplished through a combination of full–time university and NRC personnel on–site at the CEWES MSRC, in close communication with completely dedicated university personnel dividing time between the CEWES MSRC and the university, and with faculty members at the university with partial time commitment to the CEWES MSRC PET effort for support and leadership.

The university PET team for the CEWES MSRC is led by the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University, with Jackson State University as the lead HBCU/MI. The university team is as follows:

- **Center for Computational Field Simulation – ERC**
  (NSF Engineering Research Center at Mississippi State)
- **National Center for Supercomputing Applications – NCSA**
  (NSF PACI Center at Illinois)
- **Center for Research in Parallel Computing – CRPC**
  (NSF Science & Technology Center headquartered at Rice, including Tennessee)
- **Northeast Parallel Architectures Center – NPAC**
  (at Syracuse)
- **Ohio State University & Ohio Supercomputer Center – OSC**
  (at Ohio State)
- **Texas Institute for Computational & Applied Mathematics – TICAM**
  (at Texas)
- **University of Southern California**
- **HBCU/MIs: Jackson State University and Clark Atlanta University.**

Dedicated on–site/at–university support teams for each of the five DoD Computational Technology Areas (CTAs) supported at the CEWES MSRC were the responsibility of specific universities on the PET team at the CEWES MSRC in Year 2:

- **CFD: Computational Fluid Dynamics – ERC (Mississippi State)**
- **CSM: Computational Structural Mechanics – NCSA (Illinois) & ERC (Mississippi State)**
- **CWO: Climate/Weather/Ocean Modeling – Ohio State**
- **EQM: Environmental Quality Modeling – TICAM (Texas)**
- **FMS: Forces Modeling and Simulation/C4I – NPAC (Syracuse)**

as were each of the following three technical infrastructure support areas:

- **Scalable Parallel Programming Tools – CRPC (Rice/Tennessee)**
- **Scientific Visualization – NCSA (Illinois)**
- **Collaboration/Communication – NCSA (Illinois)**

Mississippi State, Texas, and Rice maintain on–site university personnel at the CEWES MSRC in support of CFD (Dr Steve Bova – MSU), CSM (Dr Rick Weed – MSU), EQM (Dr Bob Fithen – Texas) and Scalable Parallel Programming Tools (Dr Clay Breshears – Rice), and NCSA at Illinois has a dedicated person spending significant time on–site in support of Scientific Visualization (Dr Alan Shih). Ohio State has a dedicated person spending significant time on–site in support of CWO (Dr David Welsh); and OSC has an on–site person supporting Computational Migration (Mr Trey White). NRC has a person on–site in support of Scientific Visualization (Dr Richard Strelitz – SAIC). NRC also has a Training Coordinator (John Eberle – NRC) and a PET Webmaster (Hermann Moore – E–Systems) on–site.

Since the great majority of users of the CEWES MSRC are off–site, the PET effort at the CEWES MSRC places emphasis on outreach to remote users through visits to major remote user sites, training courses at such remote sites, web–based remote training delivery, and remote communication via email and the CEWES MSRC PET website. Central to this outreach to all users is a CEWES MSRC User Taxonomy that has been prepared and is maintained by the CEWES MSRC PET team in order to understand the user distribution and needs. During Year 2, the CEWES MSRC PET team was in direct contact with over a hundred CEWES MSRC users at twenty–two sites. The CEWES MSRC PET team had over eighty person–days in contact with MSRC users at the annual DoD HPCMP User's Group Meeting. In addition to the permanent on–site component of the CEWES MSRC PET team, other members from the team universities accumulated a year and a half of person–days on–site at CEWES MSRC.

Training is the most visible part of the PET program for many of the CEWES MSRC users. During Year 2, a total of twenty training courses were conducted, seven of which were at remote user sites. Service to remote users was also improved by completion of the Training and Education Facility (TEF) at CEWES MSRC. The TEF is furnished with professional–quality video production and recording equipment. Training material from any source (laptop, workstation, transparencies, etc.) can be projected onto the classroom screen for instruction, broadcast over Mbone, and saved on videotape. Material from the training courses is posted on the CEWES MSRC PET website:

http://apollo.wes.hpc.mil/

During the Fall 1997 and Spring 1998 terms, Jackson State University, in Mississippi, twice offered the course CSC 499, "Programming for the Web" to its students in connection with the CEWES MSRC PET effort – with the course being taught by instructors physically located at Syracuse University in New York using materials developed for use in regular Syracuse courses. The technology behind this distance education project is the Tango collaboratory tool and the WebWisdom educational repository and presentation tool, developed by Syracuse utilizing Java and other web–based technologies to provide an environment for the full two–way exchange of multimedia content in real time. This partnership between Jackson State and Syracuse also served as a pilot for the use of the Tango and WebWisdom tools to deliver CEWES MSRC PET–sponsored training classes to DoD researchers.

The enhancement of the programming environment at CEWES MSRC through the identification and introduction of programming tools, computational tools, visualization tools, and collaboration/information tools is a major emphasis of the CEWES MSRC PET effort. Twenty–five such tools were introduced into CEWES MSRC by the PET team during Year 2, and training courses at CEWES MSRC and at remote user sites for many of these tools were provided, along with continual guidance and assistance in their use through the on–site team at CEWES MSRC. In addition, five grid generation systems were installed. The CEWES MSRC PET team conducted twenty–one specific focused efforts during Year 2 in connection with this effort to evaluate, implement, and enhance such tools for introduction into CEWES MSRC.

An evaluation of currently available grid codes (COTS, freeware, and research codes) was conducted by the PET team at CEWES MSRC, and a workshop on the utility of grid generation systems for CEWES MSRC users was held – targeted specifically at five "grid–related" CTAs: CFD, CSM, CWO, EQM, and CEA – in order to assess user needs and to formulate strategy to address needs not being met by available grid systems. This grid workshop also served to broaden the awareness of the availability of grid generation resources to the CEWES MSRC user community.

Assistance in migration of codes to the T3E, SP, and O2K was provided to CEWES MSRC users by the PET team both directly and by providing tools and technology to the CEWES MSRC Computational Migration Group at CEWES MSRC. The PET team also worked with CEWES MSRC users to enhance algorithms, physics, and visualization in user codes in the CTA areas supported at CEWES MSRC, with specific impact on eighteen CEWES MSRC user codes during Year 2.

The leadership of the CEWES MSRC PET team was active in interaction with the DoD CTA Leaders and in MSRC–wide coordination during Year 2, participating in the Timberline meeting with the CTA Leaders and responding to their White Papers outlining needs in the CTA areas that might be addressed by the PET program across the MSRCs, and participating in the Rice meeting of the PET leadership across the MSRCs.

During Year 2, the CEWES MSRC PET team included 122 people from 10 universities. The team made direct contact with 103 CEWES MSRC users at 22 sites, and had 472 person–days on–site at CEWES MSRC in addition to the permanent on–site members. There were 42 person–days of travel to conduct remote training for CEWES MSRC users, and 145 person–days of travel to meetings and workshops directly related to the CEWES MSRC PET effort. And there were 227 person–days of travel to national meetings for presentations related to the CEWES MSRC PET effort, to meet CEWES MSRC users, and to track technology developments in the interest of the CEWES MSRC PET effort. The CEWES MSRC PET team had direct impact on 18 codes in use at CEWES MSRC, and introduced 26 programming, computational, visualization, and collaboration tools, and 5 grid generation systems, into CEWES MSRC. The CEWES MSRC PET team carried out 22 specific Focused Efforts during Year 2 to enhance the programming environment at the CEWES MSRC.

A total of 13 training courses covering 37 days, were conducted on–site at CEWES MSRC, and 7 courses covering 23 days were conducted at 2 remote user sites. These training courses were attended by 45 CEWES MSRC users from CEWES and 97 from other CEWES MSRC user sites. A workshop for grid systems across five CTAs was conducted, with 42 attendees from all four MSRCs and two DoE labs, including representations from five grid–related CTAs: CFD, CSM, CWO, EQM, CEA. Five training courses or seminars were conducted at the HBCU/MI member sites of the CEWES MSRC PET team: four at Jackson State and one at Clark Atlanta, impacting over 170 students and faculty from these and three other HBCUs. Two regular semester undergraduate courses were conducted at Jackson State over the web, and one graduate course was conducted at CEWES. The CEWES MSRC PET team produced 40 CEWES MSRC/PET technical reports, 23 conference presentations, and 6 journal papers reporting on PET efforts of Year 2.

URL: http://apollo.wes.hpc.mil/

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I. INTRODUCTION

1. The DoD High Performance Computing (HPC) Modernization Program (HPCMP)

The Department of Defense (DoD) High Performance Computing (HPC) Modernization Program (HPCMP) was instituted in 1994 to modernize the total high performance computational capability of the military research, development, test, and evaluation (RDT&E) community to a level comparable to that available in the foremost civilian and other government agency RDT&E communities. A key component of this initiative is the DoD Major Shared Resource Centers (MSRCs).

The MSRCs provide complete HPC environments and include various types of computing systems, scientific visualization capabilities, extensive peripheral and archival storage, and expertise in use of these systems. The MSRCs support the wide variety of research and development problems arising from the science and technology programs supporting DoD's weapons development and warfighting support systems. The MSRCs provide the computer and computational sciences expertise to allow all of the DoD laboratories to advance their capability in science and technology. The types of computer systems in the MSRCs are determined by user requirements and differ from one MSRC to another.

The HPCMP selected four DoD sites to become MSRCs:

- **Army Corps of Engineers Waterways Experiment Station (CEWES), Vicksburg MS**
- **Army Research Laboratory (ARL), Aberdeen Proving Grounds MD**
- **Naval Oceanographic Office (NAVO), Stennis Space Center MS**
- **Air Force Aeronautical Systems Center (ASC), Wright–Patterson AFB, OH**

In addition, DoD has identified ten Computational Technology Areas (CTAs) as being critical across all of DoD. These ten CTAs supported by the MSRCs are:

- **CFD: Computational Fluid Dynamics**
- **CSM: Computational Structural Mechanics**
- **CCM: Computational Chemistry and Materials Science**
- **CEA: Computational Electromagnetics and Acoustics**
- **CWO: Climate/Weather/Ocean Modeling**
- **SIP: Signal/Image Processing**
- **FMS: Forces Modeling and Simulation/C4I**
- **EQM: Environmental Quality Modeling**
- **CEN: Computational Electronics and Nano–Electronics**
- **IMT: Integrated Modeling and Testing**

An integral part of the DoD HPCMP is the provision of Programming Environment & Training (PET) at each of the MSRCs by university/industry teams in order to enable DoD researchers to develop and utilize the necessary HPC software. The PET program includes training courses in all aspects of HPC in the Computational Technology Areas (CTAs) and in relevant programming and technical infrastructure areas. And it includes side–by–side transitioning of research codes into the MSRCs, as well as collaboration with MSRC users to advance and improve those codes.

The DoD HPCMP and the MSRCs are described more fully at the HPCMP website:

http://www.hpcmo.hpc.mil/

2. The Programming Environment & Training (PET) Program

The Programming Environment & Training (PET) component of the DoD HPC MSRCs is a bold and innovative approach to enhancing the capability of the MSRC users comensurate with the enhancement of the power of the hardware in the MSRCs, in order to realize the expressly stated goal of the DoD HPC Modernization Program to attain a level comparable to that in the foremost university, industry, and other Government agency HPC centers. The PET effort provides the essential user support and mode of capability enhancement that is necessary for the MSRCs to attain this goal – and to address the wide variety of research and development demands arising from the science and technology programs supporting DoD's weapons development and warfighting support systems.

The purpose of the PET component of the MSRCs is to enhance the entire programming environment for the MSRC users through training and support for software enhancement, addressing both near–term improvements and long–term expansions, thus enabling use of the MSRC computing resources to fullest capacity and extending the range of applicability of HPC to DoD technical problems.

The PET component of the MSRC program is thus a true intellectual enterprise which breaks new ground in collaborative effort between DoD and academia in order to establish a two–way conduit of information and expertise enhancing the capability of the MSRC user and bringing demands of DoD HPC to bear early–on in programming environment developments in progress in the universities. The PET effort is unprecedented in its concept and vision, in its management for long–term achievement, in its strong university commitment, in its approach through unique university/DoD collaboration, in its understanding and relationship between university researchers and MSRC users – and in its challenge posed in the interest of DoD to the universities and companies involved, the MSRC users, and the program management.

The PET team at the CEWES MSRC has now completed its second year of effort, and that is the subject of this report. The approach of this report is to collect complete data and item lists on all aspects of the Year 2 PET effort of the CEWES MSRC into a series of tables, so that the text can concentrate on a narrative of the operation and accomplishments of the effort. More complete and continually updated information on the current PET effort of the CEWES MSRC is accessible on the CEWES MSRC PET website which is reachable from the CEWES MSRC website:

http://apollo.wes.hpc.mil/

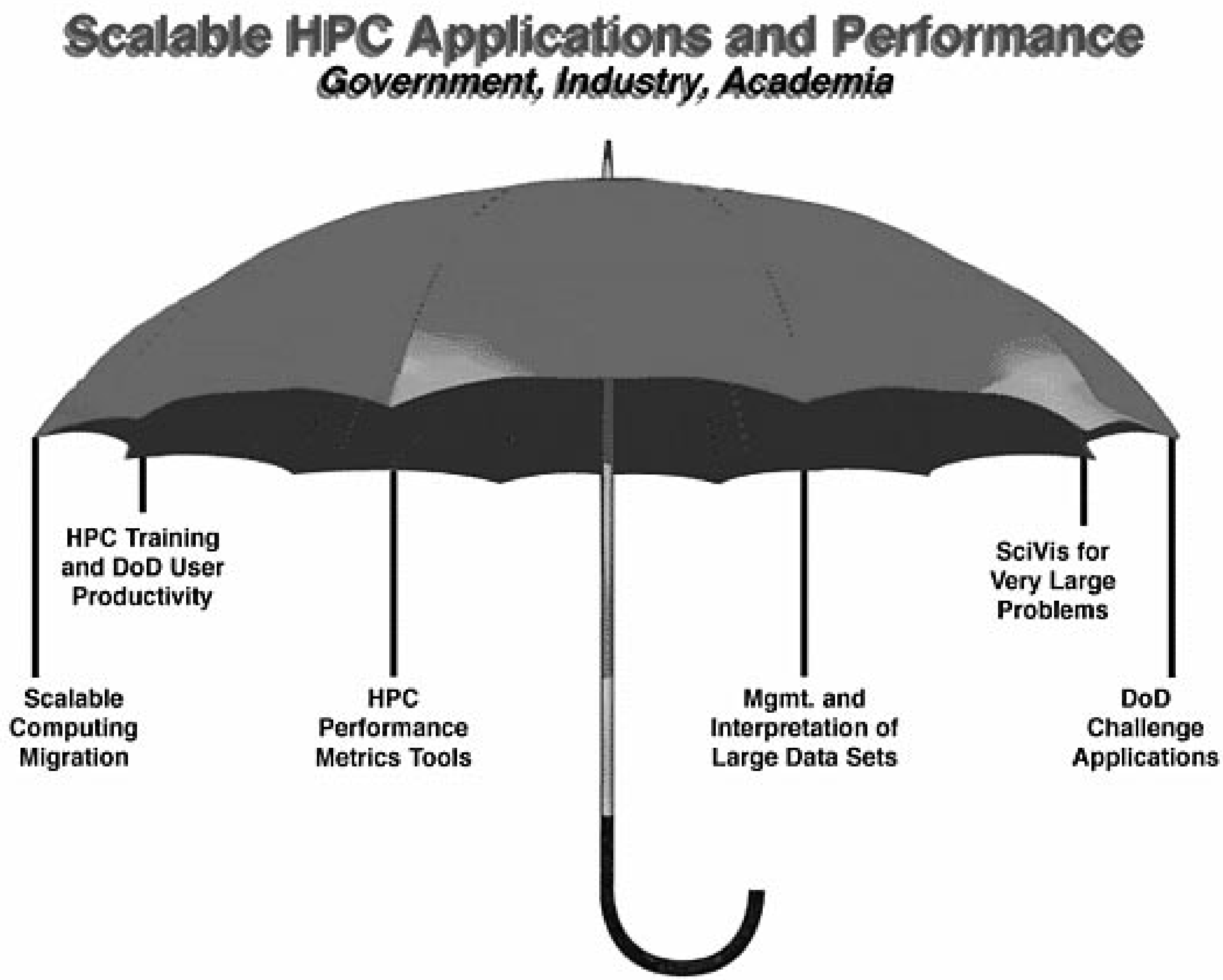
After discussing the strategic plan for the CEWES MSRC PET effort and its general implementation in Sections II and III, the specific organization of the CEWES MSRC PET support structure is described in Section IV. Major accomplishments of the PET effort at CEWES MSRC during Year 2 are presented in Section V, with the continuing vision given in Section VI. Of particular impact are the tools introduced into the CEWES MSRC covered in Section VII. The training component of the CEWES MSRC PET effort is a major means of transfering technology to CEWES MSRC users, and this component is reported in Section VIII. Further specific discussion of outreach to CEWES MSRC users, both on–site and remote, appears in Section IX. The HBCU/MI element of the CEWES MSRC PET effort in Section X is especially important in that it serves to enhance the capability of HBCU/MIs in high performance computing and in the ability of these institutions to produce future researchers in this area. Finally, a complete list of publications arising from the PET effort at the CEWES MSRC is included. An Addendum gives summaries of each of the specific focused efforts conducted by the PET team of the CEWES MSRC during Year 2.

II. CEWES MSRC PET STRATEGIC PLAN

The strategic plan of the CEWES MSRC PET effort has evolved over the first two years of operation, through close collaboration of the university team leadership with that of Nichols Research and the CEWES MSRC.

1. Goals and Objectives

The goal of the PET effort at the CEWES MSRC is to bring university HPC knowledge and skills to bear on both the overall theme – Scalable HPC Applications and Performance – and the specific sub–areas listed as examples under the "umbrella" for the CEWES MSRC:



CEWES MSRC Vision "Umbrella"

The key objectives of the PET effort in the CEWES MSRC are as follows:

- **Establish a mechanism for identifying and transfering emerging advances in programming environments, computational tools, algorithms, and computational solution techniques for CTA applications from academia and industry into the CEWES MSRC.**
- **Create a virtual extension of the CEWES MSRC into academia that will be responsible for identifying and acquiring near–term programming environment improvements and long–term expansions, anticipating CEWES MSRC user needs and making users aware of pertinent emerging technology.**
- **Utilize state–of–the–art HPC technology as an inherent part of the implementation of the CEWES MSRC PET Program itself.**
- **Establish a training program to ensure CEWES MSRC user proficiency with transfered advances in HPC tools and technology.**
- **Establish cooperative development and training programs with HBCUs/MIs to significantly enhance participation in the HPC community.**
- **Establish effective collaboration with academia to encourage the development of graduate and post–doc programs that will enhance the skill levels and efficiency of the DoD HPC community.**

Based on this, the vision for PET at CEWES MSRC is to:

- **Transfer cutting edge, innovative HPC technology and tools from premier university centers to CEWES MSRC users and laboratories.**
- **Provide innovative collaborative environments for HPC research to all CEWES MSRC users (“remove importance of place”).**
- **Train CEWES MSRC users in state–of–the–art HPC and scalable parallel processing (SPP) programming tools and techniques.**
- **Use HBCU/MI partners in an integral way to support PET objectives, enhance faculty and train minority students in HPC.**
- **Enable CEWES MSRC to make major productivity gains from current/planned hardware acquisitions in PL1/2/3.**

The true deliverable of the CEWES MSRC PET effort is the raised level of CEWES MSRC user capability and programming environment in the CEWES MSRC – to a level not surpassed by academic, industry, or other government HPC centers.

2. Approach

The approach to PET at the CEWES MSRC is to marshall an elite and readily accessible university team to constitute a virtual extension of the CEWES MSRC into top academic expertise, able both to respond and anticipate needs of the CEWES MSRC users for training and assistive collaboration in advancing the programming environment, utilizing a combination of strong on–site presence and dedicated support from the universities.

Support for CEWES MSRC users is provided by the PET team in the five Computational Technology Areas (CTAs) for which the CEWES MSRC has responsibility:

- **CFD: Computational Fluid Dynamics**
- **CSM: Computational Structural Mechanics**

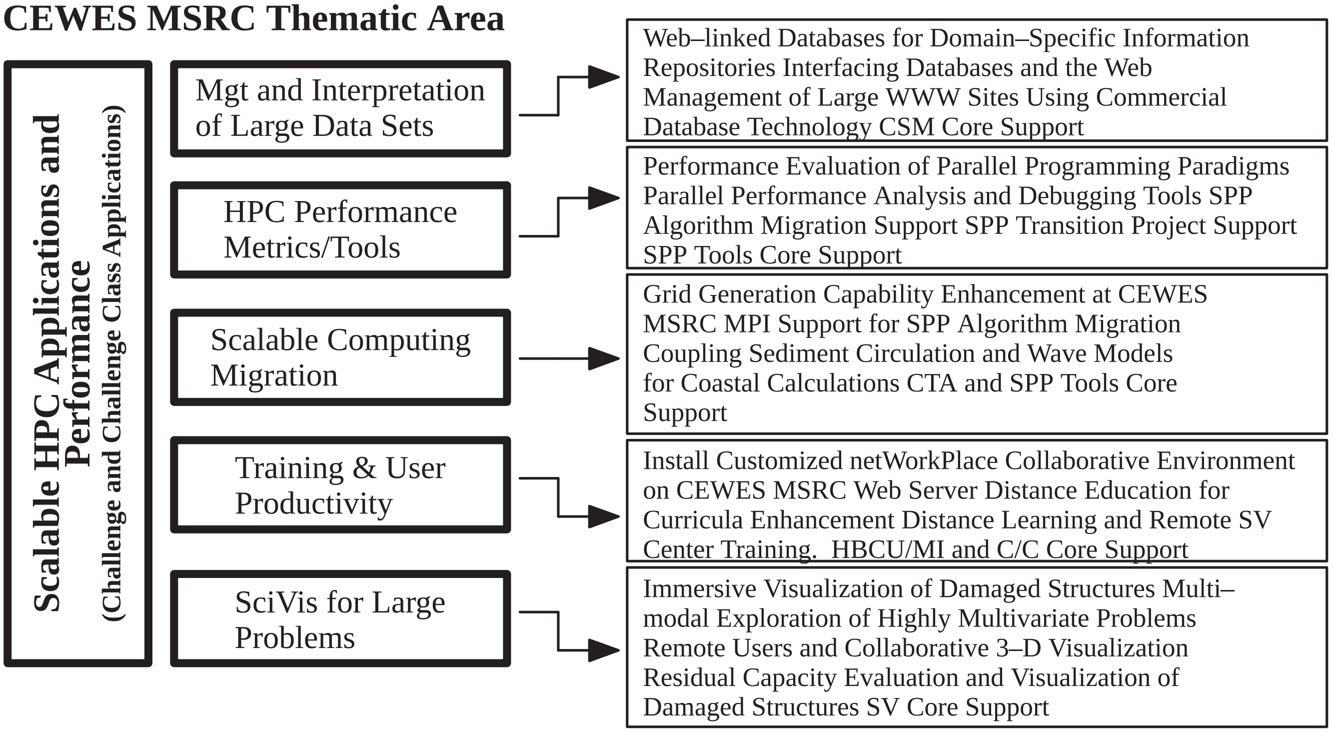
- **CWO: Climate/Weather/Ocean Modeling**
- **EQM: Environmental Quality Modeling**
- **FMS: Forces Modeling and Simulation/C4I**

and also for three relevant technical infrastructure areas:

- **Scalable Parallel Programming Tools**
- **Scientific Visualization**
- **Collaboration/Communication**

The PET effort at CEWES MSRC consists of three fundamental elements: Core Support, Focused Efforts, and Training. Intertwined with these efforts are outreach to CEWES MSRC users and a program to enhance the involvement of HBCU/MIs in HPC.

CEWES MSRC Thematic Area



Core Support provides continual interaction and assistive collaboration with CEWES MSRC users in the technical areas supported at the CEWES MSRC to migrate and enhance important codes to scalable parallel platforms and to extend the applicability of such codes and systems.

Focused Efforts address current specific projects to enhance the programming environment at the CEWES MSRC and the capabilities of CEWES MSRC users.

Training provides instruction for CEWES MSRC users, both on–site at CEWES MSRC and remote, in the technical areas supported at the CEWES MSRC and consists of both in–person and web–based courses.

3. Core Support

Core Support is provided to the CEWES MSRC through continual interaction in each of five CTAs supported at the CEWES MSRC, as well as in the three technical infrastructure support areas, with a specific supporting university on the PET team having responsibility for each area.

This Core Support operates primarily on–site at the CEWES MSRC, coupled with continual support from specific individuals at the university, through continual interaction and assistive collaboration of the PET team with CEWES MSRC users in the five CTAs supported at the CEWES MSRC, and in the three technical infrastructure support areas, to migrate important codes to scalable parallel platforms and to enhance and extend the applicability of such codes and systems. In the operation of this Core Support, CEWES MSRC user demographics and software usage are continually monitored to provide input for identification of codes and systems of important impact.

4. Focused Efforts

In addition to this continual Core Support, certain specific Focused Efforts within the scope of the CEWES MSRC and the resources of the PET effort are identified for implementation by the CEWES MSRC PET team, operating across the universities as necessary. Such projects have specific objectives and deliverables. When appropriate, projects involve coordinated efforts among PET teams from other MSRCs and/or funding from other MSRC PET efforts. Interest by CEWES MSRC users in collaborative effort in such projects is a necessary factor in identification of such Focused Efforts for implementation.

5. Training

Training is conducted with emphasis on intermediate and advanced topics, and is coordinated across the MSRCs to reach the entire DoD user community. A state–of–the–art training facility is maintained at the CEWES MSRC with workstations for hands–on training and facilities for remote transmission. Delivery is on–site at the CEWES MSRC, in–person at some other DoD sites and at the universities as appropriate, and remotely using emerging distance learning approaches. Training specifically addresses the need to reach an ever greater number of DoD users, leveraging emerging digital infrastructures and the unique educational expertise of the CEWES MSRC PET team. Delivery is ultimately to be any time, any place, and at any pace.

6. Outreach

Since the great majority of users of the CEWES MSRC are off–site, the PET effort at the CEWES MSRC places emphasis on outreach to remote users through visits to major remote user sites, training courses at such remote sites, web–based remote training delivery, and remote communication via email and the CEWES MSRC PET website. Emphasis is also placed on the implementation of appropriate tools for remote collaboration, especially with regard to scientific visualization. Continually updated user demographics are assembled into a CEWES MSRC user taxonomy to guide this outreach to all users of the CEWES MSRC.

7. HBCU/MI Program

The principal purpose of the HBCU/MI component of the PET effort at the CEWES MSRC is to enhance the capability of the HBCU/MI members of the CEWES MSRC PET academic team to participate fully in the PET support effort of the CEWES MSRC. To this end, both Jackson State and Clark Atlanta are involved directly in Focused Efforts. Particular emphasis is placed on enhancing the opportunities of students at the HBCU/MI PET partners through web–based university classes at the HBCU/MIs from the other PET team members and through summer institutes at the HBCU/MIs.

III. IMPLEMENTATION

1. Management

The CEWES MSRC PET effort is administered by the integrator, Nichols Research Corporation (NRC), for the CEWES MSRC as a part of the CEWES MSRC contract. Dr Dick Pritchard of Nichols Research is the PET Director. Dr Joe Thompson of Mississippi State University is CEWES MSRC PET academic team leader. Dr Wayne Mastin of Nichols, and a professor emeritus of Mississippi State, is the on–site PET team leader. Dr Willie Brown of Jackson State University is the HBCU/MI leader. Dr Louis Turcotte of the CEWES MSRC exercises oversight of the CEWES MSRC PET effort for the government.

2. Organization

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3. Team Composition

The university PET team for the CEWES MSRC is led by the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University, with Jackson State University as the lead HBCU/MI. The university team is as follows:

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as also were each of the following three technical infrastructure support areas:

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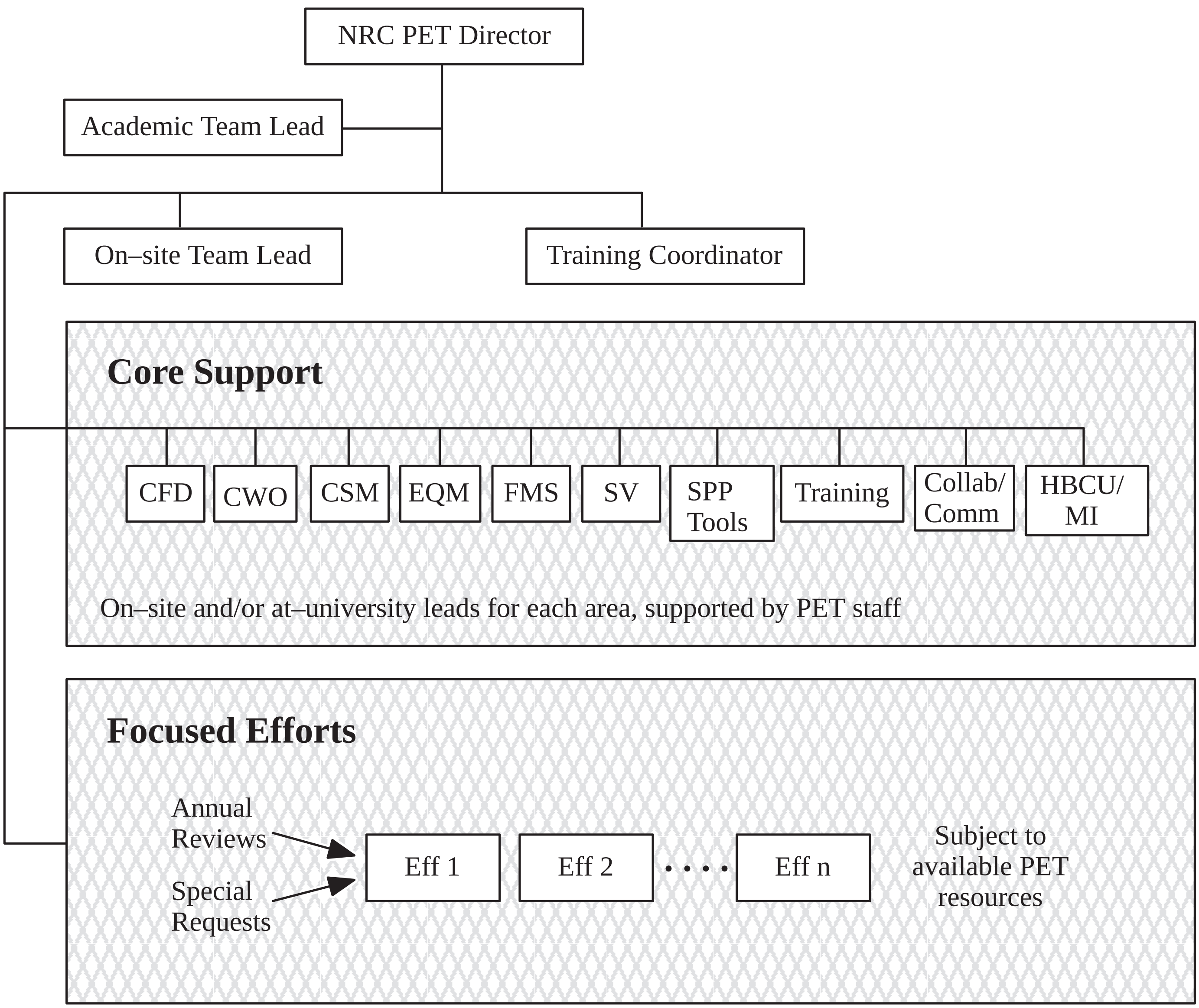

PET Organizational Structure

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4. Reporting and Technology Transfer

Transfer of emerging technology from the academic community into the CEWES MSRC is a primary purpose of the CEWES MSRC PET effort. Of like importance is transfer in the other direction, providing input and feedback regarding emerging DoD needs to influence developments at universities. The primary mode of technology transfer in the CEWES MSRC PET effort is direct contact between the PET team and the CEWES MSRC users. But the PET team also produces a series of reports on technology developments for distribution to CEWES MSRC users. And technology transfer is a prime emphasis of the training component of the CEWES MSRC PET effort. The on–site personnel at the CEWES MSRC from the PET team form a continual conduit for technology transfer.

5. MSRC–wide Coordination

MSRC–wide coordination is led by the PET Executive Committee (ExComm), which was formed during the Year 2 effort. The ExComm is chaired by Ken Kennedy of Rice, and includes the academic leaders for the PET effort at the four MSRCs:

- **CEWES MSRC: Joe Thompson – Mississippi State**
- **ASC MSRC: Charlie Bender – Ohio State**
- **ARL MSRC: John Toole – Illinois**
- **NAVO MSRC: Andrew Grimshaw – Virginia**
- **HBCU/MI: Willie Brown – Jackson State**
- **scribe Chuck Koelbel – Rice**

The ExComm conducted a meeting in September 1997 of the DoD CTA Leaders and the PET leaders from all universities involved at the four MSRCs. And the ExComm produced, during Year 2, a collective response of the PET teams of all four MSRCs to the White Papers from the DoD CTA Leaders indicating needs in the CTAs that might be addressed by the PET effort. Finally, the ExComm has produced a vision statement for the PET effort, together with White Papers in five technical areas essential to the effort:

- **Metasystems**
- **Programming Tools**
- **Application Tools**
- **Scientific Visualization**
- **Training & Collaboration**

These are all at the ExComm website: http://www.crpc.rice.edu/DODmod/index.html.

It is imperative in the interest of efficiency of resource utilization that the PET support teams for the four MSRCs move to coordinate their efforts and cooperate as much as is feasible in view of the differing emphasis and user patterns, and in view of the fact of separate contracts. Collaboration should not, however, be an end in itself, but rather coordination should operate to bring expertise and developments to bear across the MSRCs. Where possible, resources are leveraged by obtaining agreements with the PET efforts at other MSRCs to jointly fund appropriate projects.

IV. TECHNICAL SUPPORT TEAMS

The fundamental mode of operation for PET support at the CEWES MSRC is a direct and continual connection between the CEWES MSRC PET team universities and the CEWES MSRC users in support of the five Computational Technology Areas (CTAs) supported at the CEWES MSRC and three related technical infrastructure areas.

This is accomplished through on–site PET team members at the CEWES MSRC in close communication with PET team members at the supporting universities, who also make frequent visits to CEWES MSRC. The PET team members on–site at CEWES MSRC are full–time university personnel, supplemented by full–time NRC personnel. Some of the PET team members at the universities are full–time in the PET effort, spending regular time on–site at CEWES MSRC. The on–site PET team members at the CEWES MSRC are key to the CEWES MSRC PET operation, since these team members are the front line of contact with CEWES MSRC users. These six on–site team members now are:

- **Lead: Dr Wayne Mastin – NRC (Professor Emeritus of Mississippi State)**
- **CFD: Dr Steve Bova – Mississippi State**
- **CSM: Dr Rick Weed – Mississippi State**
- **EQM: Dr Bob Fithen – Texas**
- **SPPT: Dr Clay Breshears – Rice**
- **SV: Dr Richard Strelitz – NRC (SAIC)**

Also on–site at CEWES MSRC are the PET Director, Dr Dick Pritchard, and the Training Coordinator, John Eberle, both of NRC, and the PET Webmaster, Herman Moore of E–Systems. During most of Year 2, Dr Carey Cox of NRC was on–site in support of CWO, but has now left for an academic career. A complete listing of all the CEWES MSRC PET team personnel is given in Table 1.

A total of 122 people from ten universities were involved in the CEWES MSRC PET effort during Year 2. Of these, 29 are PhDs. Three were located on–site at CEWES MSRC, all PhDs: two from Mississippi State, and one from Rice. A fourth, from Texas, is now in place. In addition, NRC had five on–site in the CEWES MSRC PET effort. And fourteen graduate students and two undergraduates were involved at the universities on the PET team.

During Year 2, the eight technical support teams in the CEWES MSRC PET effort operated as follows:

CFD: Computational Fluid Dynamics CTA

CFD support in the PET effort at CEWES MSRC, as well as at the ASC and ARL MSRCs, is the responsibility of the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University. At the beginning of Year 2, the CFD support team consisted of Dr David Huddleston (academic leader) and Dr Jianping Zhu at Mississippi State, with Dr Steve Bova of Mississippi State on–site at the CEWES MSRC. As the year progressed, the team was supplemented by the addition of Puri Bangalore at MSU for MPI support and Clarence Burg (graduate student). Although Mr Burg made valuable contributions, his financial support was leveraged from another MSU project, and no CEWES MSRC PET resources were expended for his direct financial support.

The on–site leader (Bova) serves as a highly–effective liaison between CEWES MSRC, NRC and MSU and as a technical liaison between CEWES MSRC users and the entire CFD support team. During Year 2, the CFD team duties evolved such that Bova now coordinates communication and facilitates interaction with other components of the CEWES MSRC PET team. This includes maintenance of the CFD webpages and biweekly activity reporting.

The CFD team in the CEWES MSRC PET effort serves the CEWES MSRC by providing

a. Program–wide CFD support.

b. R&D expertise on selected technology enhancements.

c. HPC assistance for targeted codes.

The program–wide support pertains to direct CEWES MSRC user contact and cultivation, participation in workshops and technical meetings, user training in HPC, and other generic duties. HPC support for targeted codes and delivery of collaborative R&D expertise are more specific tasks selected to produce technology that has potential application and interest throughout the CEWES MSRC user community.

CSM: Computational Structural Mechanics CTA

PET support for the Computational Structural Mechanics CTA at the CEWES MSRC was provided in Year 2 by NCSA (National Center for Supercomputing Applications) at the University of Illinois, under the leadership of John Towns (acting Academic Lead) and LeRay Dandy (CSM Project Team Leader), together with on–site support of structural codes of importance to CEWES MSRC users in CSM and visualization support for these users. The on–site support was provided by Dr Rick Weed of the ERC at Mississippi State, in communication with NCSA, and the visualization support was provided by NCSA.

The team also included project engineers at NCSA, including Dr Cristina Beldica (tracking and web support), Dr Bruce Loftis (CSM Visualization), Youngjin Woo (graduate student) and Gyuseok Kwak (graduate student). Dr Fouad Ahmad served as CSM Academic Lead for part of Year 2. At Clark Atlanta University, Dr O. (Tido) Olatidoye, Dr S. Sarathy and students C. McIntyre and G. Jones were also involved.

The primary focus of the CEWES MSRC PET CSM team is to increase CEWES MSRC user productivity of widely–deployed DoD codes. Productivity increases are realized by developing software tools and methods which automate time–consuming processes often encountered within the CSM project cycle. In addition, the CSM team provides the best available solutions for specific problems encountered by users.

CWO: Climate/Weather/Ocean Modeling CTA

PET support for the Climate, Weather and Oceanography CTA at CEWES MSRC is provided by The Ohio State University, Department of Civil and Environmental Engineering and Geodetic Science, under the leadership of Dr Keith Bedford. The co–project lead is Dr P Sadayappan of the Department of Computer and Information Science. The CWO team consists of Dr Shuxia Zhang, Dr David Welsh, and Sean O'Neil. Dr Carey Cox of NRC served as the on–site CWO leader until January. Welsh spends time on–site at CEWES MSRC, and is responsible for working with CEWES

MSRC personnel in the wave and circulation modeling activities. Zhang is a research scientist responsible for the focused effort work and continues to work with personnel in CFD on the CH3D–SED and MM5 models. O'Neil is a graduate student working on circulation modeling. All staff share in programmatic responsibilities including interaction with CEWES MSRC personnel, other CEWES MSRC PET team activities and MSRC–wide responsibilities, especially with NAVO MSRC.

EQM: Environmental Quality Modeling CTA

PET support for the Environmental Quality Modeling CTA at the CEWES MSRC is provided by TICAM (Texas Institute for Computational & Applied Mathematics) of the University of Texas at Austin, under the leadership of Dr Mary Wheeler. The support team for the EQM effort includes Drs Wheeler, Clint Dawson, Victor Parr, Srinivas Chippada, Carter Edwards, Monica Martinez, and Robert McLay; and graduate students Sujatha Sagiraju, Joe Eaton, and Jennifer Proft. Staff members include Connie Baxter, Sarah Woodruff and Stephanie Tomlinson. Wheeler is the technical area leader, and Dawson is co–leader.

Parr is a scalable programming expert and has also acted as a virtual on–site person. He is in frequent contact with the CEWES MSRC users. He has been primarily involved in the parallelization of CE–QUAL–ICM and more recently ADCIRC. Chippada and Proft have also been involved with CE–QUAL–ICM. Martinez has joined the team to help with the parallelization of ADCIRC. Edwards and Eaton have provided software support (i.e., a mesh partitioning algorithm) for both of these projects. Sagiraju, Bryant and McLay have been involved in the development of a web launching capability for the ParSSim code. Wheeler, Dawson, Edwards, Martinez and Parr also participated in the Parallelization Technology Workshop held at CEWES MSRC in January 1998. Baxter, Woodruff and Tomlinson provide staff support and webpage support.

FMS: Forces Modeling and Simulation/C4I CTA

The Northeast Parallel Architectures Center (NPAC) at Syracuse University has the lead role in FMS support at both the CEWES and ARL MSRCs, under the leadership of Dr Geoffrey Fox. NPAC's support team for the FMS area is composed primarily of NPAC's Interactive Web Technologies Group, lead by Dr Wojtek Furmanski. NPAC has extensive experience in both HPCC and commodity technologies, such as the World–Wide Web, Java and related tools, CORBA, and DCOM, as well as modeling and simulation. The Interactive Web Technologies group is comprised of more than a dozen researchers working on a variety of synergistic projects. Group members focusing especially on activities related to the CEWES MSRC PET program include graduate research assistants Ozgur Balsoy, Hasan Ozdemir, and Zeynep Ozdemir.

The Forces Modeling and Simulation CTA is in a fairly unusual position among the DoD CTAs, though it does share some characteristics with Integrated Modeling and Testing (IMT). Both FMS and IMT tools are widely used throughout the DoD; however only a very small portion of the user base is HPC users. Instead, for a variety of reasons, most FMS computing is done using local workstation or PC resources. To further complicate the situation, this field is in the midst of a transition from the well–established "distributed interactive simulation" standards for the development of applications to the new object–oriented "high–level architecture" (HLA) approach, following the mandate of the Defense Modeling and Simulation Office (DMSO).

Supporting a field in this situation is somewhat of a challenge. The approach adopted by the PET program (at both the CEWES and ARL MSRCs, where FMS is supported) involves tracking and monitoring this complex and changing field and its relationship to commodity and HPCC technologies. A small number of carefully chosen focused efforts are used to demonstrate the convergence of HLA with commodity distributed computing technologies, and to migrate applications with substantial HPC requirements to such systems. The overall goal of this approach is to develop exemplars which can then be used to highlight to the MSRC user community the opportunities available through the use of HPC and commodity technologies.

SPPT: Scalable Parallel Programming Tools

The SPP Tools support team is based at the Center for Research on Parallel Computation (CRPC), an NSF–funded Science and Technology Center with headquarters at Rice University. Rice plays the lead role in SPP Tools at CEWES MSRC, ARL MSRC, and ASC MSRC. The University of Tennessee at Knoxville (UTK) is also a key CRPC site, and has a major role in SPP Tools at CEWES MSRC. The goal of the CRPC is “to make parallel computing truly usable by scientists and engineers”. Toward this end, CRPC researchers have attacked the software and algorithmic problems posed by parallel and distributed machines. The solutions they have identified are crucial elements in the DoD HPC Modernization Programming Tools effort.

Individually, the SPP Tools support team includes internationally–recognized experts in the areas of distributed and parallel computing, dense and sparse linear algebra, parallel languages and compilers, parallel benchmarking and performance evaluation, and interprocessor and network communication. Team members have considerable experience in producing, deploying, and supporting software systems that turn their best research ideas into widely used tools, such as the Parallel Virtual Machine (PVM) system and the ScaLAPACK parallel linear algebra library. In addition, team members have led a number of significant standards efforts, including the High Performance Fortran (HPF) Forum, the Message Passing Interface (MPI) Forum, the BLAS Technical Forum, and ParkBench. They have also been instrumental in transferring technologies, including compiler data dependence analysis and memory hierarchy optimization techniques, to the commercial sector. Some of the key personnel involved in CEWES MSRC PET are Dr Ken Kennedy (Senior Technical Lead, Rice University), Dr Jack Dongarra (Senior Technical Lead, UTK), Dr Chuck Koelbel (SPP Tools Lead, Rice University), Dr Shirley Browne (SPP Tools Lead, UTK), and Dr Clay Breshears (On–Site SPP Tools Lead). Nearly a dozen additional PhD–level researchers also participate at Rice and UTK.

The primary goal of SPP Tools is to promote a uniform, high–level, easy–to–use environment for programming available to all CEWES MSRC users and, ultimately, to all of DoD. We view “programming” very broadly, encompassing any means of describing a sequence of executable actions. This includes writing traditional CFD simulations as well as developing quick–and–dirty filters to scan output files. Similarly, we view “tools” as including any software that eases the task of programming. This includes tools, such as compilers, that make programming possible at all; it includes other tools, such as libraries, that provide easier–to–use facilities for programming; and it includes some tools, such as performance profilers, that help users understand their programs. In order to move toward this goal, we emphasize several secondary objectives:

a. Promote efficient, abstract programming. We work to supply languages and systems programmed in terms near the problem domain, and automatic tools that produce efficient machine–level programs. Since such systems are still some way in the future, we also work to improve lower–level languages and tools to provide short–term help to CEWES MSRC users.

b. Enhance program understanding. We consider tools that collect static and/or dynamic data, relate the data to the original program, and assist the programmer in improving the program. Out of necessity, we also consider currently available tools that do not meet all of these criteria.

c. Establish standards for a uniform programming environment. We promote this by seeking out and promoting high–quality implementations of formal and informal standards, and by helping to develop new standards as technology matures.

SPP Tools is a cross–cutting area: if we are successful, all CTAs will benefit from the new tools. It has a long–term goal that will not be met by PET activities alone; in order to provide a complete set of tools, far more resources will be needed than DoD Modernization alone can provide. We therefore put great emphasis on collaboration with CEWES MSRC users (to understand the requirements for new tools), with other CEWES MSRC PET team members and other MSRC PET teams (to disseminate and test the tools), and with groups outside of DoD (to identify and develop the tools).

SV: Scientific Visualization

PET support for Scientific Visualization at the CEWES MSRC is the responsibility of NCSA (National Center for Supercomputing Applications) at the University of Illinois, under the leadership of Dr Polly Baker. The CEWES MSRC PET Visualization team includes the Senior Academic Lead (Dr Polly Baker from NCSA), an on–site NRC Lead (Dr Richard Strelitz from SAIC), and an NCSA Lead (Dr Alan Shih from NCSA). Dr Baker provides long–term direction and leadership for the effort. Dr Shih serves as the primary conduit between activities at NCSA and the CEWES MRSC. He is headquartered at NCSA and spends a significant amount of his time on–site at the CEWES MSRC. Dr Strelitz is located at the CEWES MSRC and works closely with Dr Shih. Milti Leonard and Edgar Powell of Jackson State University are also involved.

The team also includes project developers at NCSA, such as Randy Heiland, Dave Bock, and Rob Stein. Ed Peters is a graduate student involved in project development. Alan Craig provides tracking and web support, along with two undergraduate students, Tom Devor and Nate Crane. In the summer of Year 2, the team also included Dr Jay Jackson, serving as the NCSA Lead.

The CEWES MSRC PET SV team interacts with CEWES MSRC users to define user needs, provide information on available solutions, and prototype custom solutions where necessary. The team also coordinates with other CEWES MSRC personnel specializing in visualization. For example, we share information and tools with visualization developers at the CEWES MSRC. We also team with the local visualization specialists on selected development projects, such as the Chesapeake Bay or Damaged Structures visualizations. Activity in support of Scientific Visualization in the CEWES MSRC PET effort is characterized by a combination of efforts intended to apply to a broad user community at the CEWES MSRC, as well as efforts that support a particular user group.

C/C: Collaboration/Communication

Support for the Collaboration/Communication technical infrastructure on the CEWES MSRC PET team is provided by NCSA (National Center for Supercomputing Applications) at the University of Illinois and the Northeast Parallel Architectures Center (NPAC) at Syracuse University.

NCSA made transitions in this team in Year 2, from Dr John Ziebarth to Lex Lane as Senior Lead, and from Frank Baker to Sandie Kappes as Team Leader. Lisa Gatzke is the Web Developer. In addition to the NCSA staff, Herman Moore (E–Systems) is the CEWES MSRC PET Webmaster.

Dr Geoffrey Fox leads the overall C/C effort at NPAC. Database–related activities were handled primarily by Dr David Bernholdt and Yuping Zhu, while work on the Tango collaboratory system and related tools was lead by Dr Marek Podgorny. The Tango group also included Research Scientists Roman Markowski, Tomasz Jurga, Tomasz Major, Konrad Olszewski, Piotr Sokolowski, Rawel Roman, Tomasz Stachowiak, Remek Trzaska, and Bart Winnowicz as well as Graduate Research Assistants Lukasz Beca and Grzegorz Lewandowski.

V. YEAR 2 ACCOMPLISHMENTS

As has been noted, the PET effort at the CEWES MSRC operates through providing core support to CEWES MSRC users, performing specific focused efforts designed to introduce new tools and computational technology into the CEWES MSRC, conducting training courses and workshops for CEWES MSRC users, and operating an HBCU/MI enhancement program.

The major accomplishments of the CEWES MSRC PET effort in enhancing the programming environment and HPC capability of users at the CEWES MSRC are described in this present section. The presentation here is according to CTAs and technical infrastructure support areas, but there is much overlap in effort. Finally, the cross–CTA Grid Workshop conducted as part of the CEWES MSRC PET effort in Year 2 is described.

Tools introduced into the CEWES MSRC in the course of Year 2 of the PET effort are listed in Table 4, and are described in Section VII. Specific CEWES MSRC codes impacted by the PET effort during Year 2 are listed in Table 5, and items of technology transfer into the CEWES MSRC are listed in Table 6. More detail on the Year 2 effort is given in the 22 specific Focused Efforts described in the Addendum to this report. Training during Year 2 is described specifically in Section VIII, and specific outreach to CEWES MSRC users in Section IX. The accomplishments in the HBCU/MI component of the CEWES MSRC PET effort are covered in Section X. And lists of CEWES MSRC PET technical reports and publications are included following Section X.

During Year 2, the CEWES MSRC PET team included 122 people from 10 universities. The team made direct contact with 103 CEWES MSRC users at 22 user sites, and had 472 person–days on–site at CEWES MSRC. There were 42 person–days of travel to conduct remote training for CEWES MSRC users, and 145 person–days of travel to meetings and workshops directly related to the CEWES MSRC PET effort. And there were 227 person–days of travel to national meetings for presentations related to the CEWES MSRC PET effort and to track technology developments in the interest of the CEWES MSRC PET effort. The CEWES MSRC PET team had direct impact on 18 codes in use at CEWES MSRC, and introduced 26 programming, computational, visualization, and collaboration tools into CEWES MSRC, as well as 5 grid generation systems.

A total of 13 training courses covering 37 days, were conducted on–site at CEWES MSRC, and 7 courses covering 23 days were conducted at 2 remote user sites. These courses were attended by 45 CEWES MSRC users from CEWES and 97 from other CEWES MSRC user sites. The CEWES MSRC PET team carried out 22 Focused Efforts during Year 2 to enhance the programming environment of the CEWES MSRC. A workshop for grid systems across five CTAs was conducted, with 42 attendees from all four MSRCs and two DoE labs, including representations from five grid–related CTAs: CFD, CSM, CWO, EQM, CEA. Five training courses or seminars were conducted at the HBCU/MI member sites of the CEWES MSRC PET team: four at Jackson State and one at Clark Atlanta, impacting over 170 students and faculty from these and three other HBCUs. Two regular semester undergraduate courses were conducted at Jackson State over the web, and one graduate course was conducted at CEWES. The CEWES MSRC PET team produced 40 CEWES MSRC/PET technical reports, 23 conference presentations, and 6 journal papers reporting on PET efforts of Year 2.

The numbers, e.g. (98–09), included with the titles refer to CEWES MSRC PET Technical Reports (TRs).

CFD: Computational Fluid Dynamics CTA
(ERC–Mississippi State)

During Year 2, the CFD team from the ERC at Mississippi State, with both on–site and at–university support in the CEWES MSRC PET effort, logged over 45 days of in–person consulting and collaboration with CEWES MSRC users through visits to CEWES MSRC and to remote user sites, visits by users to the ERC at Mississippi State, participation in CEWES MSRC technical meetings, and participation in relevant national meetings for the purpose of making further contact with CEWES MSRC users and to foster technology transfer to and from the CEWES MSRC. Numerous phone and email contacts were also made with CEWES MSRC users. The CFD team led the compilation of the CEWES MSRC User Taxonomy reported in Section IX, which serves to guide the CEWES MSRC PET team in outreach to CEWES MSRC users.

Specific technical contributions were made by the CFD team in the following categories:

a. Collation of parallel benchmarks.
b. Local support of CHSSI CFD codes.
c. Code migration assistance.
d. Development of appropriate parallel tools.

Delivery of tools and technology of immediate applicability is only one component of the CEWES MSRC PET program. We also assist CEWES MSRC users by investigating less mature technologies that have significant potential for improving DoD CFD simulation capability and applicability. Specifically in this regard, the CFD team provided individual training and worked in collaboration with DoD personnel during Year 2 to evaluate and demonstrate techniques of computational design by coupling CFD simulation capability, direct differentiation techniques, and nonlinear optimization.

Major Year 2 efforts on specific CEWES MSRC CFD user codes were as follows:

1. Demonstration of Computational Design Technology: HIVEL2D (98–09)

A free–surface incompressible Navier–Stokes solver (HIVEL2D from CEWES Coastal and Hydraulics Lab) was selected to demonstrate computational design technology. Computational design is applicable to a wide range of engineering problems relevant to DoD. HIVEL2D was selected because of general user interest within the DoD user base, because of related military engineering applications such as maintenance of dam spillways and drainage networks, and because of the technology that the code exhibits. HIVEL2D is a true finite element solver that was developed primarily for application to simulation of supercritical flows. The techniques demonstrated can, in principle, be coupled with virtually any CFD solver, and HIVEL2D thus serves as a convenient demonstration testbed.

Accomplishments included successful coupling and demonstration of direct differentiation calculation of design space gradients from the HIVEL2D solver. This is the first published example that we are aware of coupling direct differentiation concepts with a true finite element solver. The technique was demonstrated for open–channel configurations that included viscous, supercritical flow simulation. This is significant due to the complexities introduced within the direct differentiation method due to poor differentiability of fluid properties across hydraulic jumps and by CFD turbulence models. Simple design optimization examples were generated using both gradient and genetic optimization algorithms. Technical summaries of this work were provided in a CEWES MSRC technical report, a conference presentation and a CEWES MSRC seminar. Two abstracts were accepted for presentation in 1998.

2. MPI Parallelization of Hydraulic Simulation: CH3D (98–07)

During Year 2, the CFD team collaborated with CEWES Coastal and Hydraulics Lab personnel regarding parallelization of CH3D using MPI for maximum portability. The CH3D solver is a three–dimensional hydraulic simulation code that has been used to model various coastal and estuarine phenomena. It is a complex, legacy code with more than 18,000 lines. The code is capable of handling highly irregular geometric domains involving coastlines and rivers and has been widely used by the Army Corps of Engineers for both hydrodynamics simulations and as a foundation for many of the environmental quality and sediment transport models, as well as for remediation of land around DoD bases, environmental impact studies, ensuring waterways remain navigable, etc. As such, the reduction of execution time of CH3D is critical to various DoD hydrodynamics simulations and environmental quality modeling projects.

This collaboration has been successful in that we have been able to (1) provide specific HPC support and training to a major CEWES MSRC user, (2) develop CH3D expertise that enables use as an HPC test and evaluation platform, and (3) utilize CH3D as a mechanism to promote collaboration with the CWO and EQM CTAs in the CEWES MSRC PET effort.

The initial MPI parallelization of CH3D was completed in 1997. Numerical experiments verify that the results for velocity, water surface elevation, salinity, and temperature distributions from the parallel code are identical to results from the sequential code (16 digits using free format output in Fortran). Almost every subroutine in the original code was modified. More than 2000 lines have been added to the code for parallelization. The execution time has been significantly reduced using multiprocessors. For example, a simulation that would have taken five days to finish on a single processor can now be done in just one day using seven processors.

There are a large number of legacy production codes written in Fortran for vector computers. The data structure, controlling logic, and the numerical algorithms in these codes are in general not suitable for parallel computers. The parallelization work on CH3D not only reduces the execution time for this particular code, but also provides valuable experience on migrating other complex application codes with similar data structures and numerical schemes from vector computers to parallel computers.

Year 2 efforts helped to improve the parallel efficiency by reducing memory usage, minimizing interprocessor communication and maintaining good load balance. Collaboration with the CWO and EQM teams was initiated to integrate hydraulic, sediment transport, and wave models for large–scale simulations. It is also planned, as a long–term goal, that different numerical integration algorithms will be tested and compared with the ADI–type scheme used in the CH3D code, and a better scheme will be developed and implemented in CH3D to further improve its efficiency on parallel computers.

3. Assistance with CHSSI Codes: OVERFLOW and FAST3D

Immediate HPC assistance was provided to CEWES MSRC users by direct collaboration on targeted codes. Contacts were made with each of the CHSSI CFD teams, with varying levels of interaction established. We expect to continue and expand this effort in Year 3. Particularly successful collaborations have been established with the CHSSI OVERFLOW (Army Aeroflightdynamics Directorate at NASA Ames Research Center) and FAST3D (NRL) development teams. In this regard, we provided the FAST3D team with the first implementation of their code on an IBM SP. Similarly, we assisted the OVERFLOW team with their first implementation of OVERFLOW–D1 on a Cray T3E.

4. Evaluation of Parallel Programming Models (98–32, 38)

There is an ongoing effort in the CFD team to evaluate the trade–offs associated with the various parallel programming models which are available. We are using two DoD codes as testbeds for this investigation. More specifically, we are collaborating with CEWES MSRC users David Medina of AF Phillips Lab and Fernando Grinstein of NRL. Medina has a Smooth Particle Hydrodynamics (SPH) code – MAGI – which is used by the Air Force for hypervelocity impact studies. We have assisted him with optimizing a shared memory version using PCF directives on the CEWES MSRC Origin 2000. We have also assisted him with an HPF implementation, and have developed a Fortran binding for the Posix Pthreads standard in an attempt to further optimize the shared memory version. We feel that it is important to investigate the feasibility of the Pthreads model for high–performance parallel computing. Grinstein has a three–dimensional chemically reacting Navier–Stokes code – TURB3D – which is used by the Navy for investigating mixing phenomena associated with noncircular jets. We are assisting him in developing a scalable parallel version of TURB3D. In this case, both MPI and HPF approaches are being used to evaluate the relative merits of each tool within the context of an actual DoD application.

CSM: Computational Structural Mechanics CTA
(NCSA–Illinois & ERC–Mississippi State)

Year 2 support of the CSM CTA at CEWES MSRC consisted of on–site support of CTH and Dyna3D codes for simulation of damaged structures, provided by the ERC at Mississippi State, and Focused Efforts performed by NCSA at Illinois which included

a. Developing an Dyna3D–to–EPIC translator.

b. EPIC Optimization on the SGI Origin 2000.

c. Developing a tool to monitor CTH simulations while running on a high performance computer.

In addition, the on–site CSM lead assisted in the coordination of the SciVis effort for the Damaged Structures Challenge Project and supported the Grid Capabilities Enhancement Focused Effort and the grid workshop by coordinating the acquisition and evaluation of CSM–related grid codes.

Specific effort on Computational Structural Mechanics tools for the CEWES MSRC during Year 2 follows:

1. On–Site Support for Damaged Structures Challenge Project: CTH and Dyna3D

The on–site CSM lead, Rick Weed, provided support for Raju Namburu's (CEWES) Damaged Structures Challenge Project by assisting with the resolution of problems encountered with the CTH code. Visualization support of this same CSM effort was provided by NCSA. This visualization support of CSM is discussed below as the second item in the Scientific Visualization part of this section.

2. Dyna3D–to–EPIC Translator

DoD scientists use both Dyna3D and EPIC for analysis of CSM problems involving large deflection of structures with material nonlinearities. EPIC has similar functionality, with special emphasis in the area of projectile impact and penetration. Dyna3D input has become a standard for this type of analysis and is easily produced by many pre–processors. A Dyna3D–to–EPIC translator has been delivered by LeRay Dandy of NCSA at Illinois to CEWES MSRC users which will allow models to be created in Dyna3D format and subsequently translated to EPIC format with minimal user intervention.

3. EPIC Optimization on Origin 2000

EPIC is increasingly being used for projectile impact and penetration problems by CEWES MSRC users. Most EPIC runs are on a single processor of the Cray C90. This machine is scheduled to be decommissioned during Year 3, which will pose a problem for EPIC users at CEWES MSRC. LeRay Dandy and Bruce Loftis at NCSA addressed the development of a parallel version of EPIC which will run on the SGI Origin 2000. A single–processor optimization of this code has been performed and has been verified using the test suite included in the EPIC distribution.

4. Monitoring CTH Simulations with CUMULVS

Simulations using codes like CTH, Dyna3D, or EPIC can take many CPU hours. Often it is not possible to discern if the simulation is progressing appropriately until the end. This effort addressed the development of a tool which will monitor specific variables during the simulation in order to allow progress of the simulation to be tracked as it is running.

CWO: Climate/Weather/Ocean Modeling CTA
(Ohio State)

Year 2 effort in support of CWO at CEWES MSRC concentrated on the physics and coupling of circulation/wave/sediment codes of interest to CEWES MSRC users, performance improvements of the wave code, and support of a major CEWES MSRC user at NRL–Stennis.

1. Deployment of CH3D, WAM and CH3D–SED (98–15)

A major focus of the Year 2 CWO effort was the coupling of circulation, wave, and sediment codes of interest to CEWES MSRC users Robert Jensen and Billy Johnson (Coastal and Hydraulics Lab at CEWES). Implementation and testing was carried out using Lake Michigan as the modeling domain. This selection simplified the specification of accurate boundary conditions, and the lake is also the site of the NSF EEGLE project, an ongoing extensive data collection program.

Three codes have been deployed for Lake Michigan :

CH3D (marine circulation model): The deployment of CH3D involved the following tasks:

a. The generation of an appropriate format grid(mesh) for Lake Michigan.
b. The modification of hardwired codings previously set for the New York Bight deployment.
c. Adaptation of the heat transfer computation to function correctly for Lake Michigan conditions.
d. Modification of the wind input codings.

We initially used the CH3D code to simulate the internal Kelvin waves and coastal upwelling fronts commonly observed in Lake Michigan. The simulation objectives were two–fold: First, to examine the capability of the modified CH3D–s (serial version) code to reproduce robust thermodynamic phenomena, and second, to tune the model’s coefficients and dynamic options to the Lake Michigan environment.

WAM (wave model): The Lake Michigan WAM deployment uses a 3–minutes longitude by 2–minutes latitude, spherical coordinate computational grid. This corresponds to approximately 4–km square cells; the dimensions of the grid are 67 cells in the East–West direction by 139 cells in the North–South direction. This grid is equivalent to the curvilinear CH3D grid. The grid's depths were resampled from the NOAA 9–arc–second Lake Michigan bathymetry database. The basic WAM deployment was tested using idealized winds to generate typical fetch–limited wave growth, sea rotation in response to wind rotation, and wave decay.

CH3D–SED (an extension of CH3D, into which a sediment module has been coupled): The sediment module computes mobile–bed processes, including aggradation and scour, bed–material sorting, and movement of bedload and suspended load of nonuniform sediment mixtures. The tasks completed for the Lake Michigan deployment of CH3D–SED were the same as those for the basic CH3D deployment. In addition, further examination was made of the suitability of the sediment transport equations. It was found that at locations where the bathymetry has a large gradient, the parameterized thickness of the active layer can be greater than that of the lowest sigma layer. It will, therefore, be necessary to calibrate and modify the sediment transport equations so that they better reflect conditions in active bedload transport regions.

2. Coupling of CH3D, WAM and CH3D–SED (98–15)

The principal reasons for coupling a marine circulation model with a surface wave model are found in the dynamic interactions taking place in the surface and bottom boundary layers of a water body. At the surface, a wave model's wave stress and radiation stress terms provide additional adjustments to water levels and mean horizontal currents in the circulation model's barotropic mode. In the wave model there will be changes due to current–induced wave refraction and unsteady depth adjustments to depth–induced refraction. The bottom boundary layer is also influenced by wave–induced bottom stresses, resulting in a feedback to both wave and current circulation models. In the bottom boundary layer, the current–induced and wave–induced bottom stresses may be directed in different, even opposing, directions and the re–suspension, entrainment and deposition processes are nonlinearly related to the relative magnitudes of the wave– and current–induced bottom stresses. Thus, properly resolving the relative magnitudes of the two stresses is important to proper application of the wave–current bottom boundary condition. So far, the wave–current interactions have been effectively coupled in the surface boundary layer. The wave–current coupling in the bottom boundary layer is being implemented in the CH3D/WAM/SED coupling system.

In order to investigate the dynamic interaction between the waves and the current circulation, we implemented both simple one–way and more sophisticated two–way couplings between WAM and CH3D, with extension of the model physics as described above. The one–way coupling was designed to isolate the individual effects of wave motion (or current) from the effects of current (or waves). The two–way coupling more realistically represents wave–current interaction by including the feedback effects due to the dynamical interactions.

The most crucial technical point in developing a realistically interactive two–way coupling lies with the synchronization of the CH3D and WAM computations at the desired time instants. This has been achieved by inserting a synchronization module into both CH3D and WAM. A series of tests has been performed for various synchronization frequencies, and the coupling synchronization between CH3D and WAM can now be performed at an arbitrary, user–specified frequency.

3. Performance Improvement of WAM (98–14)

Since WAM is a key code for CEWES MSRC users, and is very computationally intensive, optimization of its performance has been a high priority. A parallel version of the WAM code had previously been developed under a CHSSI project. The CWO PET team at CEWES MSRC has worked on improving the performance of the code. Both single–node optimization issues and parallel performance aspects were investigated.

Parallel performance optimization involved two improvements:

a. improved load balancing.

b. reduced communication overhead.

Improved load balancing was achieved through an iterative process of optimizing the choice of blocking parameters in WAM to make the number of grid points mapped to each of the processors as even as possible. The reduction of communication overhead was achieved by analyzing detailed timing traces of parallel executions to identify bottlenecks. By introducing some additional synchronization, it was possible to change the pattern of communication and improve performance. For example, a two–fold improvement in performance was achieved for the LUIS dataset on 8 processors of the SGI Origin 2000 at CEWES MSRC.

4. Optimization of the Navy Layered Ocean Model (NLOM) Model (98–14)

The Navy Layered Ocean Model (NLOM) of Allan Wallcraft (NRL–Stennis), running at CEWES MSRC, is extremely compute–intensive. One of the most computationally demanding steps in the code is that of inverting a large dense matrix. As part of CWO effort at CEWES MSRC, a parallel matrix inversion routine was deployed on the Cray T3E that resulted in significant improvement for this bottleneck computation.

The NLOM model uses a pre–processor module to compute and invert a matrix which represents the boundary conditions to be subsequently applied in the simulation module. Preliminary runs indicated that pre–processing demands were excessive. Attempts were made to improve pre–processor performance by implementing the ScaLAPACK library routines in the T3E deployment of NLOM.

ScaLAPACK is a scalable version of the LAPACK linear algebra library, built upon the PBLAS and BLACS libraries. Difficulties arose in obtaining T3E versions of ScaLAPACK, PBLAS, and BLACS which were compatible with the Cray MPI message–passing library. Complete Cray releases were not available, and the Oak Ridge National Laboratory versions designed for this application encountered problems related to differences in default data types between the T3E f90 and cc compilers. The incompatibilities were resolved by the redefinition of certain data types and the use of a special MPI flag, resulting in a consistent 64–bit package.

This implementation of ScaLAPACK resulted in significant performance enhancements. Differences between the matrices generated by the original and modified inversion procedures were consistently acceptable. Upgrades of Cray T3E ScaLAPACK and MPI libraries mean that additional efforts will be required for a stable ScaLAPACK version of the NLOM pre–processor to be secured. Ongoing work of this kind is therefore being performed by personnel at the University of Tennessee, also as part of the CEWES MSRC PET effort, as described below in the SPPT part of this section.

EQM: Environmental Quality Modeling CTA
(TICAM – Texas)

Year 2 efforts in support of the EQM CTA at CEWES MSRC were directed principally at parallization of CE–QUAL–ICM, web–based launching of ParSSim, and parallelization of ADCIRC.

1. Parallization of CE–QUAL–ICM (98–10)

Our primary effort in Year 2 was the parallelization of CE–QUAL–ICM. This project involved a close collaboration between the EQM team at the University of Texas (UT) and CEWES MSRC users, in particular Carl Cerco, Barry Bunch and Mark Noel of the Environmental Lab at CEWES. After discussions between the two groups, we decided to pursue a single program, multiple data (SPMD) approach, which would involve

a. Development of a pre–processor code which decomposes the computational domain, using a mesh partitioning algorithm, and correspondingly decomposes all global input files.

b. Modification of the ICM source code by incorporating MPI calls to pass information from one processor to another.

c. Development of a post–processor code that assembles the local output generated by each processor into global output files.

This approach to parallelization, which the UT team has used successfully on other projects, allows for scalability of the parallel computation, and hides much of the details of the parallelization from the everyday user. Scripts have been developed which the user can execute that run the pre–processor, compile and run the ICM code in parallel, and then run the post–processor. Therefore, to the user the input and output files are the same for both serial and parallel machines.

The pre–processor and post–processor codes were developed by the UT team. The pre–processor uses a space–filling curve algorithm to partition the mesh into submeshes for each processor. This algorithm is easy to implement and preserves locality of the mesh, so that subdomains with a good “surface–to–volume” ratio can be obtained.

The parallel version of CE–QUAL–ICM was developed in stages. After being given the source code by the user in early 1997, we developed a preliminary parallel code based on this version, which was completed in late summer of 1997. Simultaneously, the user was adding new features to the code, more components, new input files, etc., and these had to be incorporated into the parallel framework. This took an additional 3–4 months. By mid–December, testing began on this new code and proceeded through February.

As of late March 1998, the parallel code is being used in production mode by the user. A ten–year Chesapeake Bay simulation using 32 processors on the T3E was completed. Model calibration will be completed by mid–April and twenty–year scenarios commenced. On a single processor it was estimated that such scenarios would have been infeasible, taking over two weeks of CPU time.

2. Web–Based Launching of ParSSim

The UT team developed a web–based, code “launching” capability and demonstrated this capability on a UT parallel groundwater code, ParSSim. This simulator can handle multicomponent and multiphase flow and transport involving one fluid phase and an arbitrary number of mineral phases. It is scalable, has been fully tested, and is being employed on a collection of realistic applications.

This launching capability allows a remote user to login to a website, choose from a suite of datasets, submit a remote job on a parallel machine, and obtain graphical output of the results. A Perl script was written to drive the launching. Two groundwater remediaton data sets were constructed, which are representative of typical data sets in such problems. The ParSSim code was then executed on an IBM SP2 located at UT, on four processors. Graphical output was obtained using Tecplot and ported back to the user's machine.

A demonstration of this capability was given during the CEWES MSRC PET Annual Review in February. This effort is meant to serve as a prototype of web–based launching, which could be incorporated, for example, into the Groundwater Modeling System.

3. Parallelization of ADCIRC (98–11)

The UT team began an effort in the parallelization of ADCIRC, a shallow water circulation model used by several CEWES MSRC users (Norm Scheffner, Rao Vemulokanda, etc., of CEWES Coastal and Hydraulics Lab). The approach being taken here is very similar to the approach used for CE–QUAL–ICM. In particular, pre– and post–processors are being developed, and MPI calls are being added to the existing serial code. This development is being carried out in close collaboration with the authors of ADCIRC – Rick Luettich (North Carolina) and Joannes Westerink (Notre Dame) – who are funded through other sponsors. Our goal is to incorporate the parallelism in such a way that all future versions of ADCIRC will have a parallel capability.

The accomplishments to date include the development of a pre–processor and a parallel version of ADCIRC. These codes are being tested on a number of datasets which exercise various aspects of the simulator. The pre–processor and parallel codes execute correctly for a number of the simpler datasets. Some of the more difficult cases involve large wind stress datasets and wetting and drying. The pre–processing of wind stress data and the parallelization of the wetting and drying code are proceeding, but substantial debugging and testing remains to be done.

FMS: Forces Modeling and Simulation/C4I CTA *(NPAC–Syracuse & NRC)*

Year 2 effort in support of the FMS CTA at CEWES MSRC consisted of on–site support of a major battle simulation program (SF Express) and focused effort on run–time infrastructure by NPAC at Syracuse.

1. Battle Simulations: SF Express Demos

During Year 2, the CEWES MSRC IBM SP played a major role in two record–setting military battle simulations. This was accomplished with the assistance of the CEWES MSRC PET on–site team and the NRC infrastructure staff.

The Synthetic Forces (SF) Express application is based on the Modular Semi–Automated Forces (ModSAF) simulation engine with a scalable communications architecture running on SPPs from multiple vendors. The SF Express project is funded under the DARPA Synthetic Theater of War (STOW) program, and is supported by development teams at JPL, Caltech, and NRaD.

A record simulation of 66,239 entities, including fixed–wing aircraft, rotary–wing aircraft, fighting vehicles, and infantry was conducted on November 20, 1997, at the DoD HPCMP booth as part of the DoD contribution to the SC97 Conference. The simulation was executed by the JPL team lead, David Curkendall. The computers used for this simulation were the 256–processor IBM SP at CEWES MSRC, the 256–processor IBM SP at ASC MSRC, and two 64–processor SGI Origin 2000s at ASC MSRC, all interconnected over the DREN.

Another record was set at the Technology Area Review and Assessment (TARA) briefings at NRaD on March 20, 1998, in San Diego. Again, the CEWES MSRC SP was a major player. This simulation was conducted by the Caltech team lead by Sharon Brunett. A total of 13 computers from 9 different sites were used to host the 100,298–vehicle entity level simulation. A total 1386 processors were used in the simulation. The simulation made use of software developed in the Globus project – a research effort funded by DARPA, DoE, and NSF to investigate and develop software components for next–generation high–performance Internet computing. A list of the sites, numbers of processors, and vehicles simulated appears in the following table:

Site	Computer	Processors	Vehicles
ASC MSRC	SP	130	10,818
ARL MSRC	SGI	60	4,333
	SGI	60	3,347
Caltech	HP	240	21,951
CEWES MSRC	SP	232	17,049
HP	HP	128	8,599
MHPCC	SP	148	9,485
	SP	100	6,796
NAVO MSRC	SGI	60	4,238
NCSA	SGI	128	6,693
UCSD	SP	100	6,989
Totals		**1,386**	**100,298**

2. Object Web Run–Time Infrastructure (RTI) Prototype (98–20, 21, 22, 23, 34)

DMSO recently introduced a new integration framework for advanced simulation networking called High Level Architecture (HLA) and based on the Run–Time Infrastructure (RTI) software bus model. RTI enables federations of real–time/time–stepped and logical–time/event–driven simulations/federations, and it optimizes communication via event filtering and publisher/subscriber region/interest matching, supported by the Data Distribution Management (DDM) service.

Full and rapid DoD–wide transition to the HLA is strongly advocated by DMSO and is facilitated by open public specifications of all HLA components, extensive nation–wide tutorial programs, and prototype RTI implementations. Given the systematic shift of the DoD training, testing and wargaming activities from physical to synthetic environments, and the ever–increasing computational demands imposed on advanced modeling and simulation systems, high performance distributed computing support for HLA will likely play a crucial role in the DoD Modernization Program.

At NPAC, we are currently developing a Java–based Web Object Request Broker (WORB) server that will support HTTP and IIOP protocols, and that will act as a universal node of our HPcc (High Performance commodity computing) environment. Given that the RTI object bus model is strongly influenced by CORBA and that DMSO is in fact interacting with OMG towards proposing HLA as CORBA simulation facility/framework, an early Java/CORBA–based RTI prototype is a natural effort in the domain of interactive HLA training. Our Object Web/WORB–based RTI subset would support and integrate Web DIS (Java and VRML based) applications under development at the Naval Postgraduate School at Monterey CA, as well as more traditional and substantial simulation codes such as ModSAF and perhaps also SPEEDES, TEMPO or IMPORT, currently at the planning stage as possible FMS training targets for our PET activities at ARL MSRC.

By the end of this project, we will deliver a prototype object web (CORBA) based RTI kernel (subset) capable of running a simple demonstration application to be developed locally. This will serve as a demonstration of the integration of DMSO and web technologies and will provide a freely available tool. A follow–on project could further develop the system into a full RTI implementation, at which point it would be possible to run real RTI applications as a demonstration of this tool.

SPPT: Scalable Parallel Programming Tools *(CRPC–Rice/Tennessee, with ERC–Mississippi State)*

The SPP Tools team of the PET effort at the CEWES MSRC has mounted a coordinated, sustained effort in Year 2 to provide DoD users with the best possible programming environment and with knowledge and skills for effective use of HPC platforms. This effort can be divided into four major thrusts:

a. Working directly with users to understand requirements and provide direct help on codes.

b. Supplying essential software to meet those requirements.

c. Training in the use of that software and in parallelism issues generally.

d. Tracking and transferring technology with enhanced capabilities.

Our Year 2 effort in each of these categories is described below:

1. Working with Users: Code Migration Drives Tool Needs (98–32, 38)

A key tactic for SPP Tools is to engage users in working on their codes. It is only through such interactions that we can identify real requirements for new tools, thus ensuring that they will be relevant to CEWES MSRC. (For purposes of this discussion, we include the CEWES MSRC Computational Migration Group [CMG] as “users”: in fact, many of our closest contacts with parallel programmers are through that group.) In addition to directing future SPP Tools efforts, these interactions often lead to direct collaborations on specific codes. These have the potential for double success stories: the code improvements lead the DoD user directly to doing better science, and the lessons learned about tools provide experience for future endeavors. The latter type of success is particularly important when the user is a member of the Computational Migration Group who works with many CEWES MSRC users.

Out of many projects with users in Year 2, we mention only two. Clay Breshears, on–site SPPT lead from Rice, collaborated with members of the CMG to develop Fortran 90 bindings for Pthreads on the Power Challenge Array. In principle, the same bindings could be used on other shared–memory machines with Fortran 90 compilers; however, the detailed implementation might well differ. The importance of these bindings is that they provide a means for using fine–grain parallelism in a modern Fortran compiler. Henry Gabb of the CMG is using these bindings to parallelize David Medina’s MAGI code (AF Phillips Lab) on the PCA and Origin 2000. The relevance of the bindings extends over a wide range of potential applications. A paper on the implementation and use of the bindings will be presented at the June 1998 DoD HPC Users Group meeting.

Fortran 90 code development and testing has also been partially a user–driven activity. Breshears worked in conjunction with Steve Bova, on–site CFD leader, to produce a Fortran 90 / MPI code and an algorithm for computing shared edges on finite element grids. This is a very generic component of CFD codes, and its efficient migration to parallelism bodes well for production codes. It also illustrates the close interaction between SPP Tools and the CTA on–site team members of the PET effort at CEWES MSRC.

2. Supplying Essential Software: Parallel Debuggers, Performance Analysis (98–8, 25, 26, 27, 31, 33, 39)

To efficiently build codes, it is vital to have basic systems software available. The SPP Tools team has been active in the effort to ensure that essential system software – such as BLAS libraries, MPI implementations, and compilers – are installed on CEWES MSRC machines. These implementations are then tested and bugs are reported, so that CEWES MSRC users can build their applications on a firm foundation of properly functioning systems and library software. In particular, the SGI/Cray implementation of MPI had a number of bugs discovered in the process of installing and testing the BLACS, which underlies ScaLAPACK, on the SGI/Cray T3E.

Although correctly functioning software is necessary, correctness alone is not sufficient for effective use of HPC platforms by large–scale, computationally intensive applications. These applications also require a high level of performance from the underlying software, necessitating the development and use of benchmarks. Thus, over the past year Susan Blackford and Clint Whaley have carried out timings on a portion of the ScaLAPACK timing suite running on CEWES MSRC platforms. In addition, Phil Mucci has been active in developing a suite of low–level benchmarks for measuring application–critical performance of key linear algebra operations, of the cache and memory hierarchy, and of the communication subsystem and then running them on CEWES MSRC platforms. Gina Goff has performed similar work on a set of benchmarks to evaluate HPF constructs. The results of these performance evaluations are being made available in CEWES MSRC PET technical reports and in on–line performance data repositories, and will be presented at the June 1998 DoD HPC Users Group meeting.

As important as bringing the software to DoD sites is, it is also necessary to have a good facility for storing and announcing it. Shirley Browne and others at University of Tennessee–Knoxville (UTK) on the SPP Tools team are putting in place a repository infrastructure at CEWES MSRC that will enable sharing of software, algorithms, technical information, and experiences within and across CTAs and MSRCs and with the broader HPC community. The repository infrastructure is based on an IEEE standard software cataloging format that is implemented in the Repository in a Box (RIB) toolkit produced by the National High–performance Software Exchange (NHSE) project. Use of a standard format and of RIB provides a uniform interface for constructing, browsing and searching virtual repositories that draw on resources selected, evaluated, and maintained by experts in autonomous discipline–oriented repositories. Interoperation mechanisms allow catalog information and software to be shared between repositories. Appropriate labeling and access control mechanisms support and enforce intellectual property rights and access restrictions where needed. The repository infrastructure will facilitate easy discovery and widespread use of tools such as those described above, as well as of application codes developed by CTA teams.

As a focused effort during Year 2, Mississippi State ported the MPICH implementation of MPI onto the Cray T3E. An existing port of MPICH for the Cray T3D exists, but it is not optimal for the T3E architecture. This new port exploits the optimizations of the T3E to increase the performance of MPICH on this platform. The benefits of the MPICH port for the Cray T3E are several–fold: First, MPICH is a widely used implementation of the MPI Standard. Many programmers already use the MPI API for their code development, but an efficient port of the MPICH implementation for this platform doesn't exist. Second, since the T3E is the last in the T3 series from Cray, programmers may not want to target this platform specifically. This MPICH port gives the programmers the ability to write MPI programs on the T3E using a more optimal library implementation than previously existed on this platform. Lastly, this portable MPI code will encourage programmers and users to continue using and developing code on the T3E using MPI. The device–specific code has been written and tested using the test suite provided with MPICH. The code passes all the tests.

3. Training: Parallel Programming Techniques and Tools

Training in the use of tools, including both specific tools and general parallel programming techniques, is a vital part of our PET mission. The SPP Tools training program in Year 2 included workshops on Performance Analysis Tools, to acquaint users with software that could enhance their productivity as well as their codes; ScaLAPACK, to help users efficiently solve large dense linear systems; PETSc, to introduce users to modern template–oriented scientific libraries; and "Bring Your Own Code" workshops (often taught in conjunction with the CMG), where CEWES MSRC users have a chance to receive assistance in dealing with their individual code problems.

In the interest of brevity, we will only discuss two of the courses we offered in Year 2 (see also Table 7 and Section VIII). A highly tuned and efficient systems and library software base is essential for good application performance. However, for the results of performance evaluation studies to be of maximal benefit to DoD application developers and users, they need to be incorporated into an application performance analysis framework that provides the skills and tools needed to model, analyze, and tune application performance. To this end, UTK researchers have taught two courses in this area during the past year at CEWES MSRC – one on benchmarking and performance modeling, and one on code optimizations for MPPs. The first course shows how benchmark results can be used as a starting point and combined with application instrumentation, scalability analysis, and statistical analysis techniques to model and predict application performance on various HPC architectures. The second course covers performance optimization techniques ranging from tuning single–processor performance to tuning of communication patterns.

4. Tracking and Transferring Technology (98–2, 5)

As a comprehensive technology transfer program, the PET effort at the CEWES MSRC has a strong responsibility to evaluate and offer new technologies for DoD use. The SPP Tools team has been aggressive in both seeking out recent research and advertising it within DoD. The tools mentioned above (see also Table 4 and Section VII) are all examples of tools identified by the SPP Tools team, and their availability through RIB is a fine example of how such technologies can be made available to DoD. We mention here a few other examples of technology transfer (see also Table 6, as well as Table 4).

Because CEWES MSRC users work on multiple platforms, they need portable performance analysis tools that allow them to analyze and compare application performance on different platforms without the burden of learning a different tool for each platform. Consequently, Shirley Browne led an effort at UTK to carry out an evaluation of currently available portable performance analysis tools, including both research and commercial offerings. A CEWES MSRC PET technical report describes the results. On the basis of this evaluation, the SPP Tools team chose a handful of tools for porting and further evaluation on CEWES MSRC platforms. VAMPIR – a commercial trace–based performance analysis tool – runs on all CEWES MSRC platforms, is highly robust and relatively scalable, and has already been used to achieve significant performance improvement on a challenge application. And nupshot, a freely available trace visualization tool, has an intuitive easy–to–use interface that can quickly provide information about application communication performance. We are currently working on a robust version of nupshot and the MPE logging library that produces tracefiles for it. Furthermore, the SPP Tools team is working with developers to debug and implement Fortran 90 support for two other promising trace–based performance analysis tools, AIMS and SvPablo, as requested by CEWES MSRC users.

In the area of introducing cutting–edge research into CEWES MSRC production use, Graham Fagg and others at UTK are bringing MPI–Connect to CEWES MSRC. Although good communication performance can be achieved on a single platform by using the vendor's optimized MPI implementation, and metacomputing using MPI can be achieved using portable implementations such as MPICH, CEWES MSRC users now need the ability to couple MPI applications on multiple platforms while retaining vendor–tuned MPI implementations. To achieve this goal, the MPI–Connect system developed at UTK – which enables transparent intercommunication between different MPI implementations – is being ported to MSRC platforms and deployed to couple MPI applications in application areas such as FMS, CWO, and IMT. Without a high–level metacomputing system like this or Legion (in use at some other MSRCs), developing such multidisciplinary applications is virtually hopeless.

CEWES MSRC application developers also need the best available debugging and performance tools to enable them to quickly find and fix bugs and performance problems. However, those tools that are available have not been put into wide use for various reasons, including lack of awareness by users, poor user interface, and steep learning curves for different tools on different platforms. Ideally, a portable parallel debugging interface should be available across all CEWES MSRC platforms. Browne and Koelbel participated during the past year in a standardization effort, called the High Performance Debugging Forum (HPDF), which has produced a specification for a command–line parallel debugging interface that addresses important issues such as scalability and asynchronous control. They have solicited CEWES MSRC user input throughout the HPDF process and used it to help guide choices about what features to include and how the interface should appear. Vendor participation in HPDF indicates that the standard will be incorporated into commercial debuggers, and public–domain reference implementations are planned for the IBM SP and the SGI Origin. Thus, the efforts of HPDF promise to eventually provide a portable, easy–to–use command–line debugger for CEWES MSRC platforms.

The HPDF experience is only one of a number of efforts by the SPP Tools team to form better connections between CEWES MSRC users and the wider HPC community. Team members have attended approximately one meeting per month, publishing trip reports that have been widely circulated within DoD. Many CEWES MSRC users have commented on the value of these reports in keeping them abreast of the computational science field, even when the conference is not in their direct line of interest.

SV: Scientific Visualization
(NCSA–Illinois, with ERC–Mississippi State)

Scientific Visualization training efforts during Year 2 included development and delivery of a training course in using the new visualization package VTK (the Visualization ToolKit). This 2–day course was delivered on–site at the CEWES MSRC. Future work will include building a web–based tutorial for this package. We also directed effort toward furthering the skills of two individuals. John West, a CEWES MSRC employee currently on long–term training leave, spent the summer with us at NCSA. West worked as a member of the NCSA Visualization team on a prototype system for delivering visualization capability to users who are remote from the CEWES MSRC. Milti Leonard of Jackson State University, and a member of the CEWES MSRC PET team, worked with us at NCSA from September through December building her skills in C++ programming, HDF, and VTK. We will continue to work with Leonard. She will concentrate on techniques for supporting visualization among remote users.

Specific effort on Scientific Visualization tools for the CEWES MSRC during Year 2 follows:

1. Collaborative Visualization: VisGen (98–24, 12)

User–directed, technology–transfer efforts in Year 2 included delivering two end–user tools. The VisGen tool (currently in an alpha release) is in use by Carl Cerco and his team at CEWES Environmental Lab in analyzing data from their simulations of phenomena in Chesapeake Bay. In this work, Cerco's team models 10– and 20–year time periods, modeling concentration and transport of over 20 components (such as chlorophyll, dissolved oxygen, nitrogen, etc.). Data of this complexity could not be analyzed without visual techniques. The VisGen tool was designed and delivered to assist Cerco's team in analyzing this data. It also allows the team to capture the visualization in a web–based media, allowing Cerco to share his results with his colleagues and project managers at the Environmental Protection Agency.

2. Damaged Structures Challenge Project: Structures Visualization (98–16)

The second end–user tool is an application for viewing output from the structures codes CTH and Dyna3D. This was in support of the DoD Challenge in large–scale shock physics and structural deformation, directed by Raju Namburu of the CEWES Structures Lab. The goals of the visualization activity were to (1) provide support for this particular Challenge application, (2) highlight the science by showing the visualization at SC97, and (3) work toward advancing the methodology for managing and interpreting data from very large–scale calculations. We followed a strategy of sub–sampling the CTH data to make it more manageable, mapping that data to geometric form, and supporting interactive exploration of the playback of that geometry. Similarly, for the Dyna3D data, we extracted the region of highest interest, decimated the geometry where possible, and supported interactive playback of the geometry. To support the researchers' needs for sharing results with their colleagues, we incorporated support for image– and movie–capture. This application was used by the researchers to visually validate the results of their simulations. It was also used by the researchers to show and explain their work at SC97.

3. Visualization Toolkit: VTK

In addition to end–user tools, the SV team transferred certain technologies to the visualization specialists at the CEWES MSRC. We shared our expertise in VTK. We also made available a variety of NCSA–developed tools, including the audio development library vss, image– and movie–capture code, and a VTK–to–Perfomer utility for using VTK on the ImmersaDesk.

4. Multi–Resolutional Representation: Terascale Visualization (98–17, 18)

Preliminary investigations into terascale visualization were started in December by Raghu Machiraju of the ERC at Mississippi State, in coordination with the NCSA Visualization team. Basic investigations into the use of multi–resolutional representation for computational datasets and comparative visualization were conducted. As a result of these investigations, a journal paper was accepted for publication in a special issue of IEEE Transactions and another paper was submitted to Visualization'98. Trips to IBM TJ Watson and other companies engaged in analysis and visualization of large datasets were made to assess developments relevant to this effort. Visualization experts at DoE labs (Livermore and Los Alamos) and NASA Ames were contacted and visited. A report on terascale visualization has been prepared.

C/C: Collaboration/Communication
(NCSA–Illinois & NPAC–Syracuse)

During Year 2, the Collaboration/Communication technical infrastructure at the CEWES MSRC was supported by CEWES MSRC PET effort at both NCSA at Illinois and NPAC at Syracuse.

1. Website and Collaborative Environment: NCSA (Illinois) Efforts (98–13)

The primary objectives of the C/C effort at NCSA were to promote better information dissemination to CEWES MSRC PET users and to provide team collaboration tools for PET management and researchers. This was accomplished in Year 2 through

a. Refinement of the CEWES MSRC PET website framework and modification of the Collaboration/Communication webpages.

b. Deployment of an initial collaboration environment – netWorkPlace – enabling asynchronous postings of status reports, meetings and discussions between CEWES MSRC PET team members.

c. Building a sense of community among PET webmasters to facilitate technology transfer across the four MSRC sites.

A brief description of the activities in (a) and (c) are described in the following sections. The activities of the netWorkPlace Focused Effort project in (b) is discussed in the Addendum.

The CEWES MSRC PET website serves as a mechanism to provide timely information to users on PET program activities. NCSA developed the framework for implementing pages on the CEWES MSRC PET website in a consistent and uniform manner. This framework was developed to ensure ease of navigation throughout the site regardless of the web browser used and accessibility to visually impaired users. This framework included HTML structures for presenting frame and no–frame views of the documents as appropriate for the end–user browser software and provided recommendations for universal access considerations. Additional website support was provided through discussion with the CEWES MSRC PET webmaster, and a report was written describing website log analysis tools and how they could be used to better administer the site and to provide information to web content providers on the effectiveness of their pages.

NCSA provides website support to three of the MSRC PET sites: CEWES, ASC, and ARL. Because of the similarity of support provided to each site, it is beneficial to each site to leverage these activities across MSRCs. The mechanism chosen to support this leveraging was to build a sense of community among the MSRC PET webmasters to facilitate communication and sharing across sites. NCSA held a MSRC PET webmasters meeting in February 1998 to begin fostering this sense of community. Presentations on technology areas of interest to the webmasters were given, and discussions were held on how to foster further collaboration among the webmasters. The meeting attendees felt that the meeting was very beneficial and expressed a desire for continuation of this effort. An online discussion forum moderated by NCSA was initiated in February 1998 and has been well received by the webmasters. Additional face–to–face and online meetings will be hosted by the individual sites.

2. Tango and Search Engines: NPAC (Syracuse) Efforts (98–29)

The growth of web technologies offers some special opportunities to facilitate the work of CEWES MSRC PET team and CEWES MSRC researchers. Researchers at Syracuse University's (SU) Northeast Parallel Architectures Center (NPAC) have long been on the cutting edge of using web technology in support of high–performance computing. Tango is a Java–based collaborative tool that offers chat, whiteboard, and shared web browser capabilities, as well as two–way audio and video conferencing, which was developed previously with support from the DoD's Rome Laboratory and SU's L.C. Smith College of Engineering and Computer Science. Besides deploying Tango for a CEWES MSRC PET–supported distance education project with Jackson State University (see Sections VIII and X), NPAC researchers have also expanded the capabilities of Tango to support consulting and software development activities in geographically separated groups with the addition of a shared tool to view and modify source code as well as to debug and analyze performance.

Perhaps even more apparent than facilitating collaboration, advances in web and Internet technologies have greatly increased the amount of information which can be found on the network for a broad range of subjects. This can be an important resource for CEWES MSRC researchers, but only if it is possible to locate the desired information in the first place. To facilitate access and management of networked information, NPAC is introducing relational database systems coupled with web servers to the CEWES MSRC PET program. Initial applications include the management of large websites and the development of search engines focused on particular knowledge domains. In the latter case, a search engine focusing on grid generation (a technology cutting across several CTA areas) was developed as a prototype (see Section VII), and plans are in place for another search engine focus on Climate, Weather and Ocean Modeling (CWO) resources.

Cross–CTAs: Gridding Workshop (98–28)

As a part of the CEWES MSRC PET Year 2 effort, an evaluation of currently available grid codes (COTS, freeware, and research codes) was conducted at CEWES MSRC, and a workshop on the utility of grid generation systems for MSRC users was held at the University of Texas in Austin in February 1998. This grid workshop was targeted specifically at five "grid–related" CTAs: CFD, CSM, CWO, EQM, and CEA.

A total of 42 attendees participated in this grid workshop from all four MSRCs and two DoE labs, together with leaders or representatives from five CTAs targeted (CFD, CSM, CWO, EQM, CEA):

8 from CEWES MSRC
2 from ASC MSRC
1 from NAVO MSRC
2 from NRL
1 from LLNL
2 from Sandia
17 from CEWES MSRC PET Team
1 from ASC/ARL MSRC PET Team
1 from ARL MSRC PET Team
1 from NAVO MSRC PET Team
6 from Texas, but not PET Team

The purpose of this grid workshop was discovery and strategy:

a. Identify the needs of CTA users that are not being met with currently available grid (mesh) generation systems.

b. Formulate strategy to work with grid code developers and/or vendors to meet those needs.

The mode of this workshop was evaluation and focused discussion:

a. At CEWES MSRC, evaluate all currently available grid generation systems of potential interest to CTA users and report the results at the workshop.

b. Report at the workshop the capabilities of currently available geometry interfaces to grid generation systems.

c. Report at the workshop the capabilities of currently available domain decomposition and other parallel considerations for grid generation.

d. Hear from the CTA users at the workshop the grid–related needs that are not being met with grid generation systems now in use.

e. Through focused and directed discussion at the workshop, formulate strategy to meet the grid–related needs identified.

The development of a new grid generation package from scratch was specifically **not** a purpose of this workshop.

This grid workshop also served to broaden the awareness of the availability of grid generation resources in the CEWES MSRC user community (see Section VII).

This grid workshop focused on four specific gridding issues:

a. CAD and other input interfaces.

b. Adaptation driven by solution systems.

c. Coupling among grid systems and with solution systems.

d. Scalable parallel concerns, including decomposition.

The intent of this workshop was to compare the currently available grid generation capabilities with the identified needs of CEWES MSRC users in the "grid related" CTAs, and then to formulate a strategy to advance grid generation capability to meet those needs. This strategy may include interactions with commercial and/or research grid code developers to add features to existing grid codes or the development of add–ons, wrappers, translators, etc. for attachment to existing grid codes.

The following grid generation systems were evaluated at CEWES MSRC in this effort:

Hexahedral Codes

- **Gridgen (Pointwise Inc)**
- **GUM–B (ERC – Mississippi State)**
- **CFD–GEOM (CFD Research Inc)**
- **GridPro/az3000 (Program Development Corp)**
- **Hexar (SGI/Cray)**
- **Cubit (Sandia National Lab)**
- **TrueGrid (XYZ Scientific Applications Inc)**

Tetrahedral Codes

- **X3D (LaGrit)/GEOMESH (Los Alamos National Lab)**
- **SolidMesh (ERC – Mississippi State)**
- **VGRID/GRIDTOOL (VIGYAN Inc/NASA Langley)**

The results from these evaluations are posted on the CEWES MSRC website.

The results of this grid generator evaluation project and this workshop can be summarized as follows:

- **Current grid generation systems will generate acceptable grids about most geometries if the user is willing to spend the time required to refine the defining geometries and resulting grids.**
- **There is still not enough automation in the grid generation process.**
- **More emphasis needs to be placed on generation, analyses, and visualization of very large grid systems on parallel computing platforms.**
- **More interaction is needed between users and code developers in both DoD and DoE.**
- **More emphasis needs to be placed on the generation of large unstructured hexahedral grids of the type used in large–scale CSM analyses.**
- **There is a definite need for more support tools for the existing grid codes and some mechanism for implementing a seamless grid generation process that encompasses all phases of grid generation and geometry definition.**

VI. CONTINUING VISION

As we move into Year 3 of the CEWES MSRC PET effort, the continuing vision in the eight technical support areas is as follows.

CFD: Computational Fluid Dynamics CTA

The goal of the PET CFD team for the CEWES MSRC is to provide continual and as–required support for CFD users of CEWES MSRC, and to help develop and maintain state–of–the–art simulation capability in their application areas. Initial support projects are emphasizing efficient utilization of CEWES MSRC parallel computing capability but are not restricted to this area. We will continue to conduct collaborative research with CEWES MSRC users by

- **Assisting with the efficient utilization of CEWES MSRC computing resources.**
- **Identifying and implementing advances in simulation capability (physics, numerics, computational platforms).**
- **Dissemination of results throughout the technical community, and training and education of CEWES MSRC users.**

We have the following broad goals:

- **Leverage military applications of CFD.**
- **Make creative use of new solvers compatible with CEWES MSRC hardware.**
- **Focus on CEWES MSRC user outreach, training, and assistance to remote users.**
- **Assist CEWES MSRC users to solve complex physics in complex geometries with scalable algorithms.**
- **Guide the development of and disseminate tools for large–scale, distributed CFD visualization at CEWES MSRC.**

The CEWES MSRC PET team will provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in CFD. Targeted codes include but are not limited to the CHSSI CFD codes. Technology of interest includes CFD solution algorithms, use of parallel tools in regard to CFD codes, computational design, and grid generation in CFD. CFD support will also be provided as appropriate for migration of vector codes to CEWES MSRC scalable platforms.

CSM: Computational Structural Mechanics CTA

Rick Weed of ERC–MSU (on–site lead) will continue to support users of CTH and Dyna3D codes applied to the simulation of damaged structures, and NCSA will continue to provide visualization support of these same CEWES MSRC users. The PET team at CEWES MSRC will be expanded in Year 3 to provide a more targeted response to specific DoD requirements in CSM.

CWO: Climate/Weather/Ocean Modeling CTA

The overall goal of the CEWES MSRC PET support of CWO, which in many respects it shares jointly with aspects of EQM and CFD, is to create the algorithm, physics and computing circumstances necessary to build fully coupled atmosphere, wave, circulation and sediment transport modeling systems. Such systems will be valuable prediction tools, especially when used in forecast mode, for use in defense–related activities including harbor access for naval operations, wind–wave hazard forecasts for fleet operations, coastal condition forecasts for amphibious landing craft activities, sediment storm prediction for submarine tracking and retrieval of buried mines. The emphasis in these coupled models is on shallow and/or nearshore operations, which is complementary to the deep ocean integrated systems being implemented at the NAVO MSRC. This shallow water/coastal focus involves nonlinear and full 3D description of the physics in each code, and extremely high resolution grids with sufficient vertical resolution to predict density interfaces.

Our activities proceed in parallel with the EQM group in that their interest focuses on water quality – hydrodynamic coupling while ours concentrates on a series of couplings between physical processes. Both avenues must be pursued simultaneously as we begin to blend the coupling activities in CWO and EQM in Year 3.

To reach this goal, the following areas of development are envisioned for the next year and beyond:

1. Implementation of Robust Wave–Current Interaction Physics in the Models

To couple the wave and hydrodynamic codes with the sediment re–suspension codes for operation at the intended scales it is extremely important that wave–current interaction physics be properly included in all three models. These interactions are equally important at both the surface and bottom boundaries of the water column in the circulation and sediment codes. We will build on the terms already examined and incorporated in this year's work and include the terms for interactions at the bottom of the water column in the circulation and sediment codes.

2. Coupling of Parallel Circulation and Wave Codes and Completion of Lake Michigan Tests

Since the individual CH3D–p and WAM–p (parallel versions) codes have been parallelized during the past year, we can now complete their coupling and evaluation by application to data sets collected in Lake Michigan by the NSF–EEGLE project.

3. Parallelized CH3D–SED and COSED Models

Both the noncohesive (CH3D–SED) and cohesive (CH3D–COSED) sediment transport models must be parallelized before use in the coupled system. The OSU team is parallelizing SED, while COSED will be parallelized cooperatively with Puri Banglore of Mississippi State. Our activities here are different from the EQM transport coupling due to the fact that CH3D–SED was developed in one unified grid with one unified (and very small time step), so our coupling problem here is not cross–grid reconciliation, but rather incorporation of the physics necessary for fully coupled prediction.

4. WAM/CH3D/SED – Parallel Model Coupling and Application to Lake Michigan

With the CH3D–SED–p model scheduled for completion in mid–year three, and with our wave–current interaction coupling implemented experimentally, we expect to have a fully coupled parallel WAM, CH3D and SED system adapted and operational for Lake Michigan. Evaluation will be done using the data set mentioned above in item 2.

5. Mesoscale Atmospheric Modeling System

Here we plan on taking the first steps toward the final requirement for the fully coupled system – the implementation of a storm resolving, fully three–dimensional, mesoscale atmospheric modeling system. Until COAMPS is available to us, we will use the MM5 model developed by Penn State University and UCAR.

EQM: Environmental Quality Modeling CTA

Continuing effort in support of EQM will focus on the following:

1. Coupling of Hydrodynamics and Water Quality Models

One of the major concerns of EQM CEWES MSRC users is the coupling of simulators. For example, there are at least three different hydrodynamics codes which could in theory be coupled to the water quality model CE–QUAL–ICM. A long–term goal is to take the three–dimensional flow field from any hydrodynamic model and project it onto an arbitrary water quality model grid. Realizing such a goal is a major effort. Some of the difficulties encountered in such an arbitrary coupling are that the grids used for hydrodynamics and water quality could be very different: in particular one could be triangle–based and one quadrilateral–based. Furthermore, the velocities interpolated onto the water quality grid may not be conservative, which would lead to severe mass balance errors in the water quality model.

As a start toward realizing the goal above, we plan to investigate the coupling of ADCIRC and CE–QUAL–ICM. The difficulties mentioned above are present here: ADCIRC is based on triangles, and ICM is based on quadrilaterals. Moreover, the velocities produced by ADCIRC are not conservative, i.e., they do not satisfy the primitive continuity equations element–by–element. Thus, the coupling between the two codes will involve converting ADCIRC geometry files into ICM input files, converting ADCIRC velocity output into ICM input format, and the use of a projection method for correcting the ADCIRC velocities so that they are mass–conservative. Such projection methods have already been developed at UT but have not been applied specifically to this problem.

During the coming year we plan to develop and test the coupling of these two codes in a 2D setting, in both serial and multi–processor modes. CEWES MSRC users will be involved in the testing and validation processes. If the 2D coupling is successful, we will then proceed to full 3D models (pending the testing of 3D capability in ADCIRC).

In order to make ICM functional on more arbitrary grids, the algorithms within ICM need to be extended to triangular (prisms in 3D) type elements. Currently, the higher–order transport scheme employed in ICM works on rectangular grids, but cannot be directly extended to triangles. Therefore another long–term goal is examining the possibility of a higher–order scheme for ICM that is appropriate for triangular or other arbitrary shaped elements.

2. Web–Based Launching of Parallel Groundwater Simulations

The focus of this effort is to continue the development of web–based tools which will serve as prototypes for launching parallel simulations from remote environments. The parallel simulations of interest arise in subsurface flow and transport, but the tools to be developed will be of general use. ParSSim (Parallel Aquifer and Reservoir Simulator), a parallel, three–dimensional, flow and transport simulator for modeling contamination and remediation of soils and aquifers will be used in this demonstration. The code was developed at the University of Texas and contains many of the features of current state–of–the–art groundwater codes. It is fully parallelized using domain decomposition and MPI and is operational on the IBM–SP and Cray T3E platforms.

A client Java applet with a GUI (graphical user interface) will be developed that will allow remote users to access the ParSSim code and data domains on CEWES MSRC systems. The results of the computation are then saved on the CEWES MSRC local disks and also selectively sent back to the requesting Java applet. The Java applet can be instantiated from any Internet web browser. We will first develop appropriate tools for executing ParSSim on a single computing environment. If this proves successful, we will further investigate more complex programming tools such as Globus, which provides the infrastructure needed to execute in a metacomputing environment.

3. Parallel Visualization Capability for Hydrodynamic Flow and Water Quality Models

Visualization capability which allows the user to view solutions as they are being generated on a parallel computing platform can greatly increase CEWES MSRC user productivity through ease of debugging, ability to quickly modify input parameters, etc. VisTool, a client/server based parallel visualization tool developed by Chandra Bajaj of UT Austin, is publicly available and provides the necessary software infrastructure. VisTool visualization libraries (isocontouring, volume rendering, streamlines, error–bounded mesh decimation, etc.) are callable from Fortran and C codes, and the server side has been demonstrated on Intel Paragon and Cray parallel machines. The client side relies on OpenGL and VTK Library calls to render the application data generated by the simulation programs. Any OpenGL–capable machine (e.g., SGI, PC with OpenGL) can be used as the client machine.

Communications through client and server are performed through PVM–like communication calls. VisTool supports structured, unstructured and mixed grids, and allows both scalar and vector data to be visualized. 2D cutting planes, 1D line probes, streamlines, tracers, ribbons and surface tufts are available, and mpeg–format animations or postscript files can be generated for presentations. We will develop the appropriate interface routines which will be necessary to visualize flow and transport solution output generated, for example, by the ParSSim code.

FMS: Forces Modeling and Simulation/C4I CTA

Trends in both the military modeling and simulation (M&S) community and in the commodity distributed computing community point to the increasing convergence in the next few years of the DMSO–mandated base M&S technologies and commodity approaches involving Java, CORBA, and related tools. To highlight this convergence, NPAC (Syracuse) researchers are currently implementing HLA's Real–Time Infrastructure component in Java and CORBA. This commodity–based ”Object Web RTI” system will then be capable of supporting distributed execution of simulation applications which are compliant with HLA, while also offering the possibility to take advantage of all the capabilities of the rapidly advancing field of commodity web technologies. At the same time, the FMS support team is also investigating the Comprehensive Mine Simulator (CMS) from Steve Bishop's group at the US Army's Night Vision Directorate, Ft. Belvoir, Virginia. CMS is currently capable of handling 30,000–50,000 mines on a single processor workstation, but clearly requires an HPC system to reach the target of 1,000,000 mines.

In the near future, there will be further convergence of M&S technologies with commodity distributed computing: there is already serious discussion in the field of turning HLA into a CORBA service, for example. With this convergence, and as more FMS applications move to the HLA standard, the two aspects of the CEWES MSRC PET team's approach to the FMS field will also converge: as applications such as CMS become HLA–compliant, they can be linked into larger distributed simulations, using Object Web RTI technology to connect multiple HPCC systems together.

SPPT: Scalable Parallel Programming Tools

The SPP Tools team's plans for the future extend our current projects, always designed with an eye toward improving the overall computing environment at the CEWES MSRC. As before, these can be divided into four categories:

a. Working directly with users.
b. Supplying essential software.
c. Training in the use of that software.
d. Tracking and transferring technology.

A more detailed strategy for the Scalable Parallel Programming Tools technology area is available from the CEWES MSRC PET website. This document discusses our tactical approach.

Continuing effort in support of SPP Tools will focus on the following:

1. Working Directly with Users

The focus of our user interactions remains Clay Breshears, the Rice on–site SPP Tools lead. He is the first point of contact for any user (from DoD, contractors, or CEWES MSRC PET partners) for tools–related questions. Since most parallel programming relies heavily on tools (including libraries, runtime systems, and compilers), he is a natural point of contact for many general questions about migrating codes to or developing codes on parallel machines. Important sources of user contacts for Breshears include the CEWES MSRC "help" system, his collaborations with the CEWES MSRC Computational Migration Group (CMG), and his involvement in teaching courses. Breshears' work with users is augmented by visits from the other SPP Tools team members. Shirley Browne (Tennessee), Ehtesham Hayder (Rice), and Charles Koelbel (Rice) each have visited CEWES MSRC several times in the past and plan to continue (and increase) visits in the future.

In addition to continuing the user collaborations mentioned above, we are planning a number of new activities with CEWES MSRC users in Year 3. Perhaps most notable among these is Hayder's work on the HELIX code. This is a turbulent flow code referred to the Rice team members by the CMG. Although parallelization was working fairly well, the code suffered from below–par single–processor performance. Hayder, in consultation with other Rice University researchers, is analyzing the code for memory hierarchy pathologies and other potential problems. The CMG reports that many other codes that they examine have similar inefficiencies; while it is much too early to speculate whether the causes are similar, it is clear that we will have many targets of opportunity for applying the compiler optimizations pioneered at Rice.

2. Supplying Essential Software

Although code migration projects are helpful to the individual users of those codes, real leverage to build up an HPCMP–wide programming environment comes from supplying more generally applicable software. We will continue working closely with CEWES MSRC staff to install and evaluate potentially useful new tools. We have targeted several tools for introduction at CEWES MSRC in the next year: MPI–IO, the first portable parallel I/O interface; CAPTools, a semi–automatic parallelization tool that could significantly aid code migration efforts; and OpenMP, an emerging standard in shared–memory programming. In addition, we are tracking upgrades to several existing packages.

Although larger problems than ever before can be solved on today's scalable parallel computers, DoD users need to solve even larger problems and to couple independently developed portions of a problem running on different computer systems. This motivates an investigation of intercommunication and metacomputing technologies such as MPI–Connect, NetSolve, and SNIPE being developed at UTK, as well as the Globus and Legion systems. Specific requests by application areas for MPI intercommunication between all MSRC platforms warrants the effort to port MPI–Connect to these platforms, as well as to develop additional capabilities, such as parallel I/O for virtual file sharing.

It should also be noted that we plan to enlarge the populations of existing software repositories and add new, domain–specific repositories. Browne is spearheading this effort. The importance of these repositories is that they give a single source for users to go to obtain high–quality code, rather than continually reinventing the wheel (or, worse yet, failing to reinvent it and struggling with square wheels). This advantage has led the National Computational Science Alliance (NCSA) to adopt Repository in a Box (RIB) for their deployment mission.

3. Training

We will continue to expand the training courses offered, both by repeating popular courses (e.g. Parallel Performance Tools) and developing new ones. Some specific training plans for the next year include:

a. Involvement in the JSU Summer Institute (Koelbel, Breshears).
b. Experiences Porting Scientific Codes (Hayder).
c. OpenMP (Gina Goff).

4. Tracking and Transferring Technology

We will continue our efforts with standards efforts in the tools area, including emerging efforts like the ParaDyn/DAIS group which has recently formed. Limitations of trace–based, post–mortem performance analysis tools have been demonstrated by attempts to use them "out–of–the–box" with large–scale CEWES MSRC applications. A common platform–independent infrastructure for runtime attachment and monitoring would benefit not only performance analysis, but also interactive debugging and data visualization and would ease the task of tool writers. Such an infrastructure is being developed by the ParaDyn research group at the University of Wisconsin and University of Maryland and by an IBM parallel tools team led by Douglas Pase. The infrastructure consists of building a client–server system called Dynamic Application Instrumentation System (DAIS) on top of the low–level dyninst instrumentation library used by ParaDyn. During the next year, we plan to continue to participate in the dyninst/DAIS standardization effort and to help focus that effort by driving it with end–user tools of importance to DoD users.

We will continue to be active in the national HPC community, both to bring new, promising technologies into CEWES MSRC and to present our progress to our peers. A key part of this, as mentioned above, is attendance at conferences and professional meetings, with extensive trip reports to update CEWES MSRC users on the new technologies found there. Foremost among these is the PTOOLS Annual Meeting. PTOOLS is a consortium of users and developers who work together to build new, useful parallel tools; one of their projects was to start the High Performance Debugger Forum. Finally, Rice University is hosting the 1998 DoD High Performance Computing Users Group conference, where we will surely see many advances in the field.

SV: Scientific Visualization

In an effort to serve the overall CEWES MSRC user community in the long–term, a strategic 5–year SV plan has been developed. This SV stategic plan provides a vision for a Visual High Performance Computing environment designed to support and enhance productivity for CEWES MSRC researchers. It also provides a framework in which to organize and prioritize activities within the CEWES MSRC PET visualization program.

The SV strategic plan examines three components:

a. Anticipated changes in CEWES MSRC user needs over the 5–year lifetime of the CEWES MSRC PET effort.

b. Expected evolution of certain technologies over this time period.

c. A plan for CEWES MSRC PET efforts that will take advantage of emerging technologies to address changing CEWES MSRC user needs.

This 5–year SV strategic plan is available at

http://www.ncsa.uiuc.edu/Vis/PET/Strategy

Continuing effort in support of SV will focus on the following:

1. VisGen

The CEWES MSRC PET team's work on the VisGen tools will continue in Year 3. Extending this tool with functionality needed by Cerco's EQM group and bringing it to the maturity needed in a production–level tool is a high priority. Adapting the tool to also run on the CEWES MSRC ImmersaDesk will provide a cross–platform visual analysis tool, allowing the researcher to work on the platform best suited for the type of analysis needed. The ImmerasDesk version of the VisGen tool will also incorporate a speech interface and, eventually, audio output to augment or reinforce the visual representation.

2. Interactive Computation

The CEWES MSRC PET team for SV will also embark on an exploration of software designed to support interactive computation. Many researchers have expressed needs for the ability to monitor their simulation as it executes. This would allow a researcher to abort a run that appears to be on an unfruitful path, perhaps because of badly stated input conditions. In some cases, it might be appropriate for researchers to modify parameters of a running simulation. A variety of software, available from academia or government labs, exists to support these capabilities. The CEWES MSRC PET SV team will apply these strategies to various user codes, to be able to characterize the current support systems for computational monitoring and steering. In particular, we will apply these strategies to CTH and CE–QUAL–IQM, furthering our support for these research communities.

3. Visualization Workshop

The CEWES MSRC PET SV team in Year 3 will extend its user contact activities. We are contacting a new group of CEWES MSRC users, both on and off–site, to initiate a relationship and assess their needs. We plan to organize a Visualization workshop to share information about possible solutions with a significant number of CEWES MSRC users. Additionally, if areas are identified where existing solutions are inadequate, we can use that information to plan future CEWES MSRC PET activities.

4. Jackson State

The CEWES MSRC SV PET team will continue to work with our colleagues at Jackson State University, particularly Milti Leonard and Edgar Powell. We will continue our end–user training efforts, and will extend our offerings in web–based delivery of information on visualization tools.

C/C: Collaboration/Communication

Continuing C/C core support efforts of the CEWES MSRC PET team will focus on increased user outreach and further development of the website infrastructure to improve information dissemination. Focused efforts are planned to provide web–based training support and an intranet environment to support team collaboration. Planned outreach activities include interaction with the CEWES MSRC user community through user surveys and face–to–face meetings. Information on C/C activities and technologies will be provided through updates to the C/C webpages and seminars on technologies as appropriate. The webmaster sense of community will also be fostered through additional face–to–face meetings as well as online meetings.

Activities in the Collaboration and Communication support area will focus on expanding and enriching the information infrastructure supporting the CEWES MSRC PET team and CEWES MSRC users. General areas of effort include the CEWES MSRC PET website, and both asynchronous and synchronous collaboration tools.

The CEWES MSRC PET website is an important vehicle for the dissemination of information from the CEWES PET team to the CEWES MSRC user community. To facilitate this important function, we will participate in an initiative to increase the consistency and usability of the PET websites across all four MSRCs, thus making is easier for the content providers (the PET teams) to refer to useful information at other sites, and making it easier for users to navigate the sites and locate the information they desire from any or all such sites. We will also work on enriching the types of information that can be offered via the web site by making it easier to couple commercial databases to the web server to provide novel services such as the domain–specific WWW search engine which was prototyped this year.

Asynchronous collaboration tools, as the name suggests, are those which facilitate the interactions of groups (i.e. CEWES MSRC PET team members or CEWES MSRC users) which do not have to take place in real–time, such as a web–accessible threaded discussion space. Basic capabilities of this sort have been available at the CEWES MSRC, but have not been greatly used. We plan to promote increased use of these tools by transitioning to a new state–of–the–art asynchronous collaboration environment and simultaneously taking a more active role in studying and encouraging the use of these tools.

Synchronous collaboration tools complement other aspects of the information infrastructure, providing for real–time interaction using audio and video conferencing, shared whiteboard, and other tools. The Tango collaboratory environment was used successfully for distance education and distance consulting projects, and will now be deployed more widely for use by CEWES MSRC PET team members and CEWES MSRC users. This will be accomplished by establishing a supported and advertised Tango server at the CEWES MSRC, and by offering training classes on the Tango system.

In addition, there is a close relationship between many of the tools used in C/C and those used for asynchronous and synchronous electronic training. The C/C team will coordinate closely with activities in the electronic training area, both at the CEWES MSRC and across the PET program to help insure a consistent overall vision.

VII. TOOLS INTRODUCED into CEWES MSRC

The enhancement of the programming environment at CEWES MSRC through the identification and introduction of programming tools, computational tools, visualization tools, and collaboration/information tools is a major emphasis of the CEWES MSRC PET effort. The 26 tools introduced into CEWES MSRC by the PET team during Year 2 are listed in Table 4. The CEWES MSRC PET team has provided training courses at the CEWES MSRC and at remote user sites for many of these tools (see Section VIII), and continually provides guidance and assistance in their use through the on–site team. The purpose of this present section is to discuss the function of these tools and their importance to CEWES MSRC users. Many of these tools came from collaborative efforts across various components of the CEWES MSRC PET team, both on–site and at the universities.

I. Programming Tools

An evaluation of the state of the art in parallel debuggers and performance analysis tools has been carried out by the University of Tennessee at Knoxville (UTK), as part of the National HPCC Software Exchange (NHSE) effort. From these findings UTK was able to recommend, install, test and evaluate the utility of such tools within the CEWES MSRC user community. At present, five parallel performance analysis tools (VAMPIR, MPE logging and nupshot, AIMS, SvPablo, and ParaDyn) and one debugger (Totalview) have been made available to CEWES MSRC users on appropriate platforms. Performance analysis tools typically require the addition of code to a program (known as instrumentation) in order to write trace information to a file that will later be interpreted and displayed with a graphical interface (GUI). The purpose of such tools is to document significant events (e.g., subroutine calls, sending or receiving messages, I/O) within the execution of the user's code. Debuggers allow a programmer to examine codes as they execute in an attempt to isolate and fix catastrophic errors.

In January 1998, Shirley Browne and Clay Breshears taught a workshop at CEWES MSRC to introduce users to the performance analysis tools that were chosen for installation at CEWES MSRC. More details on each of the analysis tools and the debugger are given below, as well as work that has been done to port these tools to the various HPC machines at CEWES MSRC.

These and other programming tools are described below:

The numbers, e.g. (98–09), included with the titles refer to CEWES MSRC PET Technical Reports (TRs).

1. VAMPIR (98–02)

VAMPIR is a commercial trace–based performance analysis tool from Pallas in Germany. UTK installed, tested and evaluated VAMPIR on the Cray T3E, IBM SP and SGI Origin 2000 at CEWES MSRC. Browne and Breshears have been working with members of the CEWES MSRC Computational Migration Group (CMG) and with AFRL researchers in using VAMPIR effectively on codes of interest. VAMPIR was used with the latter group to find improvements in the communication performance of the DoD Challenge Project code ICEPIC. Browne has written CEWES MSRC PET webpages on the use of VAMPIR on the CEWES MSRC platforms.

2. nupshot & MPE Logging Library (98–02)

nupshot is a trace visualization tool that has a very simple, easy–to–use interface and gives users a quick overview of the message–passing behavior and performance of their application. nupshot analyzes trace files that are produced by the MPE logging library. Since both nupshot and the MPE (multiprocessing environment) logging library were originally designed as extensions of MPICH (the MississippiState/Argonne implementation of MPI–1), UTK has made minor modifications to the MPE logging library in order for it to work with the native MPI (Message Passing Interface) libraries on the IBM SP and SGI Origin 2000 and is currently debugging library routines which do not work properly with MPI programs that define their own communicators or topologies. A new version of nupshot was written with help from UTK that will function under multiple versions of the Tcl and TK graphics libraries.

3. AIMS (98–02)

AIMS is a freely available trace–based performance analysis tool developed by the NASA Ames NAS Division that provides flexible automatic instrumentation, monitoring and performance analysis of Fortran 77 and ASCI message–passing applications that use MPI or PVM. UTK has reported bugs in the current release of AIMS, including missing instrumentation of MPI_SendRecv and incorrect reporting of send and receive blocking times when MPI_WaitAll is used. Feedback from users at CEWES MSRC and UTK indicates that the AIMS interface, especially the source code clickback feature, is especially helpful in analyzing parallel codes. However, support for Fortran 90 would be required before this tool could realize a wide user base at CEWES MSRC. Jeff Brown at LANL has told UTK that his tools group will be adding Fortran 90 support to AIMS.

4. SvPablo (98–02)

SvPablo, another trace–based performance analysis tool, was developed by the Pablo group at the University of Illinois and is freely available. SvPablo has a GUI that lets the user determine which portions of the source code are selected for instrumentation, and then automatically produces the instrumented source code. After the code executes and a trace file has been produced, the SvPablo GUI displays the resulting performance data alongside the source code. SvPablo runs on Sun Solaris and SGI workstations and on the SGI PCA and Origin 2000. It can access and report results from the MIPS R10000 hardware performance counters on the Origin 2000. UTK has found that SvPablo has been too fragile on the CEWES MSRC Origin 2000 (it crashes frequently) to be fairly evaluated. The Pablo group claims SvPablo runs robustly on their Origin 2000 and is investigating the problem. UTK is working on porting SvPablo to the IBM SP.

5. ParaDyn (98–02)

ParaDyn, from the University of Wisconsin, is designed to provide performance measurement that scales to long–running programs on large parallel and distributed systems. Unlike the other tools that do post–mortem analysis of trace files, ParaDyn does interactive run–time analysis. For twelve or fewer processes, ParaDyn seems fairly robust. For more than twelve processes, however, it experiences catastrophic failure in about 80 percent of the runs that were attempted. ParaDyn only works in interactive mode and cannot be used on batch processing systems. ParaDyn currently runs on IBM SP systems and Breshears has been able to run the tool under an interactive batch job on the CEWES MSRC IBM SP. The developers of ParaDyn are currently working on versions that will be able to execute on other HPC machines available at CEWES MSRC.

6. TotalView

TotalView is a commercial debugger from Dolphin Interconnect Solutions that comes equipped with a GUI, but does not have a command–line interface. TotalView runs on Unix workstations, the IBM

SP and (with the newest release) on the SGI PCA and Origin 2000. TotalView for SGI IRIX 6 requires SGI MPI 3.1, but the CEWES MSRC PCA and Origin 2000 are still at SGI MPI 3.0. Browne has run TotalView successfully on the UTK SP2 which does not use PBS (Portable Batch System), but Browne and Breshears have been unsuccessful so far in getting TotalView to work on the CEWES MSRC IBM SP under PBS. Both Dolphin and Bob Henderson (developer of PBS) have been contacted about the TotalView–PBS problem. Dolphin is investigating and Henderson is willing to help from the PBS end. Since there has been considerable demand from CEWES MSRC users for a good cross–platform debugger, and TotalView has gotten good reports elsewhere, current plans are to push hard to get TotalView working on the CEWES MSRC platforms and then provide CEWES MSRC users with a one–month evaluation period.

7. MPE Graphics Library (98–05)

The MPE (multiprocessing environment) graphics library is part of the MPICH package (developed by Mississippi State and Argonne) distributed by Argonne National Laboratory as an implementation of MPI–1. This graphics library gives the MPI (Message Passing Interface) programmer an easy–to–use, minimal set of routines that can asynchronously draw color graphics to an X11 window during the course of a numerical simulation. A user can make use of the graphics routines to scrutinize the execution of code with respect to monitoring the accuracy and progress of the solution or as a debugging aid. Steve Bova and Clay Breshears were able to develop a Fortran 90 module (Fortran 90 module for parallel message passing environment [MPE] graphics) that uses these routines to draw colored contour plots for 2D unstructured grids. To this end, additional routines to draw filled triangles and polygons were written to augment the original MPE graphics library routines.

8. ScaLAPACK (98–33)

ScaLAPACK is a library of routines for the solution of dense, band and tridiagonal linear systems of equations and other numerical computations. Data sharing between distributed processors is accomplished using the Basic Linear Algebra Communication Subroutines (BLACS). The Netlib version of ScaLAPACK from UTK has been installed, tested and timed on all the CEWES MSRC platforms, and compared with vendor versions of ScaLAPACK which were also tested for correctness. Netlib ScaLAPACK has been modified to run on the SGI/Cray T3E, and a T3E patch for ScaLAPACK 1.6 is available on Netlib. Susan Blackford and Victor Eijkhout taught a training course on numerical linear algebra libraries at CEWES MSRC in June 1997. Blackford assisted Breshears in preparing webpages on use of Netlib and vendor versions of LAPACK and ScaLAPACK on CEWES MSRC platforms. ScaLAPACK has been used in the Alan Wallcraft (NRL–Stennis) Ocean Modeling DoD Challenge Project application at CEWES MSRC to achieve a significant improvement in performance.

9. PETSc

The Portable, Extensible Toolkit for Scientific Computation (PETSc), available from Argonne National Lab, is a suite of data structures and routines for the solution of large–scale scientific application problems modeled by partial differential equations. PETSc was developed within an object–oriented framework and is fully usable from Fortran, C and C++ codes. Ehtesham Hayder has installed the PETSc library on the CEWES MSRC IBM SP in order to compare the relative merits of parallel libraries versus parallel programming languages (specifically HPF) for the computational solution of numerical problems. This evaluation will help CEWES MSRC users to choose better methods for parallel computations on different parallel platforms.

10. Repository in a Box (RIB) (98–08)

Repository in a Box (RIB) is a toolkit for setting up and maintaining a software repository. It provides a uniform interface to a software catalog and facilitates interoperability, in the form of sharing of catalog information and/or software files, between repositories. RIB was used in an SC97 demonstration at the HPCMP booth of software repository interoperability between the CEWES, ARL, and ASC MSRCs. RIB is currently in production use at ASC MSRC for a CCM and parallel tools repositories. The UTK RIB installation is supporting prototype CFD (CEWES MSRC) and SIP (ARL MSRC) repositories. RIB is also being adopted by NASA HPCC sites, the National Computational Science Alliance (NCSA) and NPACI (San Diego) for their HPC software repositories.

11. Fortran Interface for Pthreads (98–32, 38)

Pthreads is a POSIX standard established to control the spawning, execution and termination of multiple threads within a single process. Use of Pthreads on a shared memory system is an attractive approach for parallel programming due in part to low system overhead. The disadvantage of Pthreads, with respect to high performance computing, is that there is no Fortran interface defined as part of the POSIX standard. We are defining and implementing a full set of Fortran 90 bindings for the POSIX threads functions. The potential impact on CEWES MSRC will be to give our users an alternative approach for higher performance shared–memory parallel programming. Breshears and Bova are using the DoD Fortran code MAGI (from the AF Phillips Lab) as a testbed for this interface.

12. MPICH on T3E (98–31)

MPICH, written by Mississippi State University and Argonne National Lab, is a portable implementation of the MPI Standard. Mississippi State University has ported this software to run efficiently on the Cray T3E architecture. Current ports of MPICH included only Cray T3D optimizations which do not run optimally on the Cray T3E. This port of MPICH to the T3E will enable the Cray T3E to join the ranks of the MPICH–supported platforms. This allows programmers to develop MPI programs on any of the supported platforms available at CEWES MSRC, easily port their programs to the various supported platforms, and exectute their programs efficiently on those platforms. This both extends the life of the Cray T3E at CEWES MSRC and increases it usefulness.

II. Computational Tools

1. Unstructured Message–Passing Toolkit (98–03)

For any finite element (or finite volume) application that solves a partial differential equation, it is necessary to partition the element mesh among the processors in order to develop a message–passing parallel implementation. Furthermore, point–to–point communication is required as a result of the local nature of the finite element approximation. If a structured mesh is used to discretize the domain, then the resulting point–to–point communication patterns are also structured and therefore straightforward to implement. Contrast this situation to that which is encountered if an unstructured mesh is used to discretize the domain. In general, each processor has a different number of neighbors with whom it must exchange data, and the length of each message can also vary. In order to manage such unstructured communication patterns, certain data must be available to the application. In particular, each processor must store the number of neighboring processors for point–to–point communication;

the destinations (origins) of the messages it sends (receives); the number of grid points along each inter–processor boundary; the identities of these grid points; arrays (buffers) in which the incoming and outgoing messages are stored; and finally, the identity of the processor in question.

The CFD team helped develop a Fortran 90 module that exploits language features such as modules, dynamic memory allocation, global variables, and user–defined data types in an attempt to bundle this data with functions in the spirit of a C++ class. This tool can provide CEWES MSRC users with a model data structure and associated functions to simplify the development of scalable message–passing software.

2. Unstructured Mesh Element Graph Finder

When partitioning unstructured grids for message–passing applications, it is often necessary to construct the graph of element connectivity. Given only an arbitrary list of elements, this tool (a Fortran 90 routine to find the adjacency list for an arbitrary 2D mesh of linear elements) returns a list, for each element, of the three (for a triangle) or four (for a quad) elements that share any edge with the element in question. It also returns a list of edges that lie on domain boundaries. The algorithm is quite fast, and computational complexity increases only linearly with the element count. This tool provides CEWES MSRC users with a robust and fast means to obtain the element connectivity graph for arbitrary, unstructured 2D meshes.

3. Grid (Mesh) Generation Tools (98–28)

As a part of the CEWES MSRC PET Year 2 effort, an evaluation of currently available grid codes (COTS, freeware, and research codes) was conducted at CEWES MSRC, and a workshop on the utility of grid generation systems for MSRC users was held at the University of Texas in Austin February 11–12 1998. This workshop was targeted specifically at five “grid–related” CTAs (CFD, CSM, CWO, EQM, CEA). The results of this Grid Workshop are discussed in Section V. (This was joint effort between the CFD and CSM teams on–site.)

The following grid generation systems were evaluated at CEWES MSRC in this effort:

Hexahedral Codes

- **Gridgen** *(Pointwise Inc)*
- **GUM–B** *(ERC – Mississippi State)*
- **CFD–GEOM** *(CFD Research Inc)*
- **GridPro/az3000** *(Program Development Corp)*
- **Hexar** *(SGI/Cray)*
- **Cubit** *(Sandia National Lab)*
- **TrueGrid** *(XYZ Scientific Applications Inc)*

Tetrahedral Codes

- **X3D (LaGrit)/GEOMESH** *(Los Alamos National Lab)*
- **SolidMesh** *(ERC – Mississippi State)*
- **VGRID/GRIDTOOL** *(VIGYAN Inc/NASA Langley)*

The results from these evaluations are posted on the CEWES MSRC website.

The CEWES MSRC offers the following grid systems to support users:

- **Hexar**
- **Cubit**
- **TrueGrid**
- **X3D/GEOMESH**
- **VGRID/GRIDTOOL**

The CEWES MSRC PET team provides instruction and guidance in the use of these systems for CEWES MSRC users.

4. Dyna3D–to–EPIC Translator

CEWES MSRC scientists use both Dyna3D and EPIC for analysis of CSM problems involving large deflection of structures with material nonlinearities. EPIC has similar functionality with special emphasis in the area of projectile impact and penetration. Dyna3D input has become a standard for this type of analysis and is easily produced by many pre–processors. A Dyna3D–to–EPIC translator has been delivered by LeRay Dandy (CSM Project Team Leader – NCSA) to the CEWES MSRC which allows models to be created in Dyna3D format and subsequently translated to EPIC format with minimal user intervention.

5. Damage Assessment and Residual Capacity Environment (DARE) (98–36)

DARE consists of several data conversion tools, modeling capability and a visualization platform. Currently interfaces to existing CHSSI SciViz tools for these components are being developed. In its present capacity these tools allow a model to be created on the CAD modeling software, and this can be migrated through a mesh generator (INGRID) to the analysis (DYNA3D) and then on to the visualization environment.

III. Visualization Tools

In Year 2, the Scientific Visualization team has contributed to the use of five new tools at CEWES MSRC. These are described briefly below:

1. VisGen (98–24)

The EQM VisGen tool supports visual data analysis for the output of the code CE–QUAL–IQM. The tool provides an easy–to–use, point–and–click interface for reading data, and displaying it in a variety of forms, including isosurfaces, colored slices, or volumes. A glyph representation is possible, to support integration of multiple variables into a single graphic. The tool supports animating through the time–series of the run.

2. Damaged Structures Visualization Tool (98–16)

The Damaged Structures visualization tool is an application that displays the output of the CTH and Dyna3D simulations, as used in the DoD Challenge Project application in simulation of building deformation in response to bomb blast. The tool supports viewing slices of the blast's pressure field or the time–series of the isosurface of the blast at 1.40e5 pascals pressure (the shock front), as well as the time–series of the building's structural response.

3. Visual Collaboration

Many CEWES MSRC researchers have expressed needs to be able to share visualization easily with their colleagues at other locations. The SV team has provided code to easily grab images and movies in a form that can be shared on the web. This code is modular and easily added to many visualization tools. It is included in both the EQM VisGen tool and the Damaged Structures visualization tool described above.

4. NCSA vss Audio Library

The NCSA vss audio library is designed to add non–speech audio to applications, particularly virtual reality applications. Audio can be particularly important in creating a sense of "presence" in a virtual environment. The vss library is based on a client–server model, and provides an API that simplifies creation and addition of audio to an application.

5. VTK (the Visualization Toolkit)

VTK, from GE Corporate Research and Development, is an increasingly popular visualization library. During Year 2, the SV team worked with our CEWES MSRC Visualization Lab counterparts to familiarize CEWES MSRC users with this toolkit. In addition to the two–day training class, we informally shared code segments, example programs, and guidance to assist CEWES MSRC personnel in building their own expertise.

IV. Collaboration/Information Tools

1. Tango & WebWisdom (98–29)

Tango is a Java–based web collaboratory developed by NPAC at Syracuse University (with funding from AF Rome Lab). It is implemented with standard Internet technologies and protocols, and runs inside an ordinary Netscape browser window (support for other browsers is in progress). Tango delivers real–time multimedia content in an authentic, two–way interactive format. Tango was originally designed to support collaborative workgroups, though synchronous distance education, which can be thought of as a particular kind of collaborative workgroup, has become one of the key application areas of the system.

The primary Tango window is called the control application (CA). From the CA, participants have access to many tools, including:

- **SharedBrowser, a special–purpose browser window that "pushes" web documents onto remote client workstations.**
- **WebWisdom, a presentation environment for lectures foilsets and similar materials.**
- **WhiteBoard, for interactive text and graphics display.**
- **2D and 3D Chat tools.**
- **RaiseHand, a tool used to signal one's desire to ask a question.**
- **BuenaVista, for two–way streaming audio and video.**

WebWisdom is a tool for showing lecture slides (or foils). Each foil may have an "addon", which is a link (or links) to supporting material such as online documentation or example programs. WebWisdom was originally developed for use in courses at Syracuse University, and was later interfaced with Tango to support the same kind of presentations to distant audiences.

Tango and WebWisdom were deployed at CEWES MSRC and Jackson State University for use in the joint Syracuse–Jackson State distance education work begun as part of the CEWES MSRC PET effort in Year 2 (see Sections VIII and X). The system was first used to present a three–day training course in the Java programming language simultaneously to a local audience at CEWES MSRC and a remote audience at JSU. Shortly thereafter, Tango and WebWisdom were used by instructors located at Syracuse to deliver full–semester academic credit courses to students located at JSU in the Fall 1997 and Spring 1998 terms. The effort has been quite successful, and with the benefit of the experience gained, expanded efforts are planned, including graduate–level course offerings, additional recipient sites, and offering CEWES MSRC PET training classes through this mechanism.

A separate effort at Syracuse focused on enhancing Tango to better support collaborative software development and remote consulting. In this project, capabilities for shared browsing and modification of source code, shared debugging, and basic shared on–line computer access were added to Tango. The new tools will be available at CEWES MSRC shortly, in conjunction with a training class to introduce CEWES MSRC users to the Tango collaborative system.

2. Grid Generation Search Engine

The ease of publishing information on the World–Wide Web has rapidly made it an invaluable source of information on a great many topics. Its popularity and the resulting growth curve has, at the same time, made it harder to sift the desired information out of the rapidly growing flood of data. Topical search engines are one way of dealing with this deluge of information. By starting from a set of "master documents", perhaps specifically identified by an expert in a given knowledge domain, it is possible to construct a specialized search engine that focuses on resources in that domain. This provides researchers with a higher "signal–to–noise" ratio in searching for focused information. Using a search engine framework previously developed at Syracuse University, this idea has been applied to produce a specialized resource on the topic of computational grid generation as part of the CEWES MSRC PET effort. This resource has the potential to benefit researchers in the various "grid–based" computational technology areas, while the underlying concept can and will be applied to a variety of knowledge domains at CEWES MSRC.

3. CEWES MSRC Search Engine

The search engine framework previously developed at Syracuse has also been used to deploy a search engine facility for the CEWES MSRC website (which includes the CEWES MSRC PET website). Based on a relational database system for high performance, the search engine can handle complex queries and return relevant documents with search terms highlighted to aid use.

4. Web Site Management System

Websites, such as those run by CEWES MSRC and the PET program, offer a sizable amount of information, with a large number of individuals contributing content. In addition, some of the information is time sensitive, as well as being subject to security review prior to release and other such concerns. The Web Site Management System is designed to streamline the routine operation of such a site by providing a famework for the management not only of the information content itself, but also the "metadata" (i.e. author, revision date, review status, etc.) which is not easily maintained or used in a traditionally–maintained website. The Web Site Management System is currently under development, and shares the same database used to support the CEWES MSRC Search Engine. The plan is to transition the system to CEWES MSRC once appropriate infrastructure is in place.

VIII. TRAINING

Training (98–01) is the most visible part of the CEWES MSRC PET program for many of the CEWES MSRC users. During Year 2, the CEWES MSRC PET training program passed several milestones. Remote classes have become a routine part of our training schedule. Service to remote users was also improved when classes moved to the Training and Education Facility (TEF). The TEF is furnished with professional quality video production and recording equipment. This has enhanced the Mbone broadcasts and improved the quality of recorded classes in the tape library. The TEF is equipped with twelve SGI Indy R5000 student workstations and an SGI O2 for the instructor. Training material from any source (laptop, workstation, transparencies, etc.) can be projected onto the classroom screen for instruction, broadcast over Mbone, and saved on videotape.

The CEWES MSRC PET training team has worked closely with Jackson State University, the lead HBCU/MI institution in the CEWES MSRC PET effort. JSU has served as a testbed and consulted on the development of the Tango collaborative environment system implemented by Syracuse University for offering remote training to off–site CEWES MSRC users.

Training Curriculum

CEWES MSRC PET training is designed to assist the CEWES MSRC user in transitioning to new programming environments and efficiently using the present and future SPP (Scalable Parallel Processing) hardware acquired under the HPCMP. The training curriculum is a living document with new topics being added continually to keep up with the fast pace of research and development in the field of HPC. The curriculum contains courses in the following general categories.

a. Parallel programming.

b. Architecture and software specific topics.

c. Visualization and performance.

d. CTA targeted classes, workshops, and forums.

Training courses are conducted both on–site at the CEWES MSRC and at remote sites with concentrations of CEWES MSRC users. Material from the training courses is posted on the CEWES MSRC PET website. Training course notices and registration are also handled on the website. Table 7 gives a list of the 20 training courses taught during Year 2, together with the evaluation score of the class on a scale of 1 (poor) to 5 (excellent). Course descriptions are included at the end of this present section.

Internet–Based Training Workshop

The CEWES MSRC PET training team was actively involved in the DoD HPC User Group Meeting in San Diego in June. CEWES MSRC PET team organized and sponsored a Real–Time Distance Training Session for the Internet–Based Training Workshop held on June 24, 1997. The purpose of the workshop was to investigate cost–effective means for providing education and training to remote users. The following presentations were given during the CEWES MSRC PET session:

- **Paradigms for Distance Education –** *Alan Craig, NCSA, University of Illinois*
- **Teaching over the Internet: A Low–Tech Approach with High–Impact Results –** *Nancy Davis, Georgia Tech*
- **CEWES MSRC Training and Education Facilities Upgrade –** *John Eberle, Nichols Research*

WES Graduate Institute

The WES Graduate Institute is an association of universities and CEWES through which academic credit and graduate degrees can be earned. The CEWES MSRC PET on–site staff supports the Graduate Institute by teaching graduate courses in high performance computing. During the Spring semester of 1997 Dr Wayne Mastin, PET On–site Team Lead, taught the MSU graduate course MA 8463, Numerical Linear Algebra. Nine students from CEWES completed the course and earned three semester hours of graduate credit from MSU.

Seminars

The CEWES MSRC PET program offers seminars at the CEWES MSRC on an irregular basis. These are presentations by experts in their field and are designed to introduce the CEWES MSRC users to current research topics in HPC. The following seminar presentations occured during Year 2 of the CEWES MSRC PET program:

- **Solution of the Time–Dependent Incompressible Navier–Stokes Equations – Numerical, Parallelization and Performance Issues**
  Dr Danesh Tafti, NCSA
  April 25, 1997
- **Java and HPC**
  Dr Geoffrey Fox, Syracuse
  July 23, 1997
- **PVMPI: Interoperating Multiple MPI Vendor Implementations with Unified Process Management**
  Graham E. Fagg,
  University of Tennessee
  October 29,1997 (JSU Seminar on October 30, 1997)
- **Scalable Computing using the Bulk Synchronous Parallel Model**
  Dr Jon Hill and Dr Bill McColl, Oxford University
  March 20, 1998 (JSU Seminar on same day)

CD–ROMS

The CEWES MSRC PET partner universities have a sizable volume of educational materials on various areas of HPCC which are suitable for asynchronous use, for example by DoD researchers wishing to increase their familiarity with various HPCC techniques and tools through self–study. NPAC at Syracuse University is leading a joint effort to produce CD–ROMs of HPCC educational material to make available to DoD researchers for self–study. The first edition of the CD–ROM includes course materials for several Syracuse University computational science courses, on–line editions of two books on HPCC, various training materials, reference material, and standards documents. Plans are to continue and expand this effort, producing at least one new CD–ROM edition each year containing new and revised materials as the HPCC landscape changes.

Web–Based Training (98–29)

During the Fall 1997 and Spring 1998 terms, Jackson State University, in Mississippi, twice offered the course CSC 499 "Programming for the Web" to its students in connection with the CEWES MSRC PET effort. The course was taught by CEWES MSRC PET team members physically located at Syracuse University (SU) in New York using materials developed for use in regular SU courses. During the regularly scheduled lectures, the instructors would display lecture slides on a workstation in Syracuse, and students attending class in a computer lab at JSU would see the slides on their screens as the instructor displayed them. The lecture was delivered through an audio link, and the students could ask questions either via the audio link or a chat tool.

The technologies behind this distance education project are the Tango collaboratory tool and WebWisdom, an educational repository and presentation tool (see Section VII). These tools, developed by Syracuse University researchers, utilize Java and other web–based technologies to provide an environment for the full two–way exchange of multimedia content in real time. Capabilities include a shared web browser, chat tool, whiteboard, and two–way streaming audio and video.

The course, which covered the architecture of the World Wide Web, HTML, CGI scripting, the Java programming language, and relational database technologies, was very well received by students. Syracuse and Jackson State are looking forward to expanding their distance education collaboration to include graduate–level courses, as well as JSU faculty teaching CSC 499 remotely to other universities. This project also served as an important pilot for the use of the Tango and WebWisdom tools to deliver CEWES MSRC PET–sponsored training classes to DoD researchers, thereby increasing the availability of classes and reducing the need to travel to attend them.

TRAINING COURSE DESCRIPTIONS

This material appears on the CEWES MSRC PET website as training course descriptions, hence the future tense.

Parallel Tools and Libraries

This course will cover parallel numerical libraries for solution of dense and large sparse linear systems. LAPACK is designed to run efficiently on shared–memory vector and parallel processors. LAPACK provides routines for solving systems of simultaneous linear equations, least–squares solutions of linear systems of equations, eigenvalue problems, and singular value problems. The associated matrix factorizations (LU, Cholesky, QR, SVD, Schur, generalized Schur) are also provided, as are related computations such as reordering of the Schur factorizations and estimating condition numbers. Dense and banded matrices are handled, but not general sparse matrices.

The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers. Like LAPACK, the ScaLAPACK routines are based on block–partitioned algorithms in order to minimize the frequency of data movement between different levels of the memory hierarchy. (For such machines, the memory hierarchy includes the off–processor memory of other processors, in addition to the hierarchy of registers, cache, and local memory on each processor.) The fundamental building blocks of the ScaLAPACK library are distributed memory versions (PBLAS) of the Level 1, 2 and 3 BLAS, and a set of Basic

Linear Algebra Communication Subprograms (BLACS) for communication tasks that arise frequently in parallel linear algebra computations.

For many large–scale scientific applications that require solving large, sparse linear systems, iterative methods are the only practical solution. PETSc, the Portable, Extensible Toolkit for Scientific Computation, is a suite of data structures and routines for the uni– and parallel–processor solution of large–scale scientific application problems modeled by partial differential equations. It includes scalable parallel preconditioners and Krylov subspace methods for solving sparse linear systems, including ICC, ILU, block Jacobi, overlapping Schwarz, CG, GMRES, and Bi–CG–stab.

Message–Passing Interface (MPI)

Message–Passing Interface (MPI) is the de facto standard for message–passing developed by the Message–Passing Interface Forum (MPIF). MPI provides many features needed to build portable, efficient, scalable, and heterogeneous message–passing code. These features include point–to–point and collective communication, support for datatypes, virtual topologies, process–group and communication context management, and language bindings for the FORTRAN and C languages. In this tutorial we will cover the important features supported by MPI with examples and illustrations. Also an introduction to extensions of MPI (MPI–2) and message–passing in real–time (MPI/RT) will also be provided.

The first day of the tutorial will be an introduction to parallel programming and Message Passing Interface (MPI) followed by discussion on point–to–point communication and collective communication. The second day will cover communicators, topologies, user datatypes, and profiling and debugging interface. On the third day we will discuss intercommunicators, extensions to MPI (MPI–2), and real–time MPI (MPI/RT) followed by an open session. Each session will have a lecture, illustration of the concepts/constructs discussed in the lecture with an example, and a lab to provide hands–on experience. Before the next session the solution to the labs will be discussed.

Performance Evaluation of Parallel Systems

This tutorial will give a comprehensive introduction to the methodology and usage of Performance Evaluation of Parallel Applications. The principles of performance evaluation will be introduced. The different levels of performance evaluation for evaluating computer systems will be introduces. These levels range from Low Level benchmarks for basic system parameters to full application benchmarks for the complete systems. The specific differences of these levels will be discussed.

The standard benchmarks for different levels of performance evaluation as well as there short–comings will be discussed in detail. This will include various standard benchmarks like the ParkBench benchmark suite, the NAS Parallel Benchmarks, the SPEC benchmark suite and the Linpack benchmark. Latest results of these standard benchmarks will be presented and analyzed.

Various issues related with workload–driven evaluation and characterization of applications and systems will be discussed. These issues will be illustrated with real application codes.

The methods for analytical performance modeling and prediction will be introduced in detail. Their application will be shown in case studies. An introduction to scalability analysis of parallel applications will be given. Different statistical methods for the analysis of benchmark results and benchmark suites will be introduced and their application to standard benchmark suites such as NPB will be shown.

T3E Applications Programming

This course is designed for applications programmers who must understand parallel processing concepts and write codes that run on CRAY T3E systems. It provides practical experience in developing, debugging, and analyzing performance of massively parallel programs using the Cray Research parallel programming paradigms and tools. No prior knowledge of parallel programming is assumed in this course.

Skills addressed:

- **Understand the CRAY T3E architecture**
- **Understand different parallel programming paradigms (message passing and shared memory routines)**
- **Demonstrate functionality in using CRAY T3E system performance analysis and debugging tools**
- **Identify the CRAY T3E I/O components**

Java and the World Wide Web

An overview of the Java language and its capabilities and the implications of Java for the World Wide Web.

Topics covered are:

- **The architecture of the Web and examples of Web/Java applications**
- **Java language basics, object–oriented programming, and animation**
- **Building user interfaces with Abstract Windowing Toolkit (AWT), I/O, and networking**

IBM SP Programming

This course will provide an overview of the features of the IBM RS/6000 SP. Students will learn the mechanics necessary to make efficient use of the machine. This course will not teach users how to write parallel programs but rather, given a program, how does one run it on the SP in an efficient and proper manner?

Students will learn about the hardware characteristics of the SP as well as the software which is available. There will also be discussion of code optimization.

Visualization Systems and Toolkits

VTK is an object–oriented system intended to provide users with a powerful yet relatively simple method for constructing visualization tools. An application written using VTK may be run on a variety of machines from PCs to workstations without modification. In addition, a user wishing to develop rapid prototypes can opt to write a VTK application which is interpreted rather than compiled as a C++ program.

This course will discuss the features and capabilities of VTK, and look at many example applications. Several labs will give participants a chance to run and modify demos. This should provide an opportunity for each to assess the potential usability of the system for visualizing data from their own area of research.

C++ Programming

The purpose of this course is teach the philosophy and syntax of the C++ programming languages. Special emphasis will be placed on two areas:

1 Improvements to the C programming language found in C++

2 The object–oriented programming features of C++

Since the object–oriented approach to writing code is a new technique for many users, the course will offer a description of and rationale for this powerful programming style.

List of Topics:

- **The class data type for object creation and use**
- **The various types of C++ functions**
- **Function and operator overloading**
- **Inheritance and class hierarchies**
- **The C++ I/O stream**
- **Abstract data types**

SGI ProDev Workshop

Speedshop/Workshop are system tools that assist the programmer in allocating memory, checking the system resources in use and are designed to assist the programmer in proficient use of the platform in use.

Parallel Programming Workshop for Fortran Programmers

The workshop will begin with a one–day lecture on strategy, tools, and examples in parallel programming. On the remaining days participants will work with their own codes.

CTH: A Software Family for Multidimensional Continuum Mechanics Analysis

CTH is a family of codes under development at Sandia National Laboratories (SNL) for use in modeling complex multidimensional (one–, two–, and three–dimensional), multi–material problems that are characterized by large deformations and/or strong shocks. A two–step Eulerian solution algorithm is used to solve the mass, momentum, and energy conservation equations. The first step is a Lagrangian step in which the computational mesh distorts to follow material motion. The second step is a remap step in which the distorted mesh is mapped back to the original mesh, resulting in motion of the material through the mesh. CTH has been carefully designed to minimize the numerical dispersion present in many Eulerian codes. All quantities are fluxed through the computational mesh using second–order convection algorithms, and a high resolution interface tracking algorithm is used to prevent unrealisitic breakup and distortion of material interfaces.

CTH has several models for calculating material response in strong shock, large deformation events. Models have been included for material strength, fracture, distended materials, high explosive detonation, and a variety of boundary conditions. The material strength model is elastic, perfectly–plastic with thermal softening, and fracture can be initiated based on pressure or principal stress. High explosive detonation is simulated using an automated programmed burn model; a Jones–Wilkins–Lee equation–of–state may be used to compute the thermodynamic properties of the high explosive reaction products. Highly accurate analytic equations–of–state may be used to model single–phase solid, liquid, and vapor states, mixed phase vapor–liquid and solid–liquid states, and solids with solid–solid phase changes.

Sophisticated graphics support is available in the CTH family of codes. A history graphics program (HISPLT) is available that allows graphical presentation of data recorded at Eulerian or Lagrangian history points during a calculation. The amount of output generated at execution by CTH is minimized, and a post processing program (CTHED) is provided that allows examination of the database at the desired times and level of detail. Finally, a very robust graphics program (CTHPLT) is available that allows graphical presentation of data in both two– and three–dimensions.

This course will present an extended overview of the features, capabilities, and usage of the CTH family of codes. Sample problems will be constructed, executed, and analyzed during interactive terminal sessions. Information will also be provided regarding ongoing CTH development activities. At the conclusion of the course, individuals should be prepared to use CTH as a tool in the analysis of realistic problems.

Techniques in Code Parallelization

The techniques needed to parallelize a code are described. These includes partitioning, load balancing, preprocessing, and postprocessing. Examples of parallelization efforts carried out at the University of Texas will be given.

List of Topics

1 Analyze Structure of the Computational Problem (Mary Wheeler)
   A. Operator Splittings and Physical Decompositions
   B. Discretization, Spatial and Temporal
   C. Solvers

2 Partitioning Algorithms and Load Balancing (Carter Edwards)

3 Data Input Integration (Victor Parr)
   A. Preprecessor for Inputs
   B. Queries for Inputs

4 SPMD Data/Domain Decomposition Formulation (Clint Dawson)
   A. Inclusion of Message Passing Libraries
   B. Interactive Visualization/Steering

5 Post–processing (Victor Parr)

Workshop on Portable Parallel Performance Tools

This workshop will cover the basics of tool–assisted performance analysis and tuning, as well as introduce a number of tools, both research and commercial, that are available on multiple parallel platforms. Both post–mortem analysis of trace files generated during program execution, and run–

time analysis using dynamic instrumentation, will be covered. Tools to be covered include AIMS, MPE logging and nupshot, Pablo, Paradyn, and VAMPIR. With the exception of VAMPIR, which is commercial, these tools will continue to be available on CEWES MSRC platforms following the workshop. (VAMPIR will be available for the week following the workshop on an evaluation license.) Workshop participants will be invited to participate in a followup usability study of the tools. Results of a preliminary evaluation of the tools may be found at http://www.cs.utk.edu/~browne/perftools–review.

Code Optimization for MPPs

This course will focus on the optimization of numeric intensive codes for MPPs. It will be a mixture of lecture and presentation with discussion and hands–on exercises in the afternoon.

The course will begin with a quick overview of the basics of performance and processor architecture. Then we will cover a wide variety of optimizations geared towards enhancing single processor performance. Topics will include efficient use of the memory hierarchy, functional units, amortizing loop overhead and dependency analysis. Common bottlenecks and caveats will be discussed as well as proposed solutions, and the logic behind them.

After covering the single processor case, we will progress towards specific optimizations geared towards MPPs. Topics will include betters ways of data layout, appropriate granularity of computation and reducing communication and contention for resources.

Lastly we will cover some details of each of the architectures in the SP, the T3E and the Origin 2000. Specific limitations of the respective architectures will be discussed as well as how they affect the various optimization techniques. In addition, each platform is shipped with programming tools designed to aid in the optimization process. The course will conclude with a quick survey of these tools and their usefulness to the application engineer.

IX. OUTREACH to CEWES MSRC USERs

Since the great majority of users of the CEWES MSRC are off–site, the CEWES MSRC PET effort places emphasis on outreach to remote users, as well as to users located on–site at CEWES. Table 3 lists the contacts made with 103 specific CEWES MSRC users by the CEWES MSRC PET team during Year 2, and Table 2 lists all travel by the CEWES MSRC PET team in connection with the Year 2 effort. A major component of outreach to CEWES MSRC users was the 20 training courses (described in Section VIII) conducted by the CEWES MSRC PET team, seven of which were conducted at remote user sites and some of which are web–based. The CEWES MSRC PET website, accessible from the CEWES MSRC website, is also a major medium for outreach to CEWES MSRC users, and all material from the training courses is posted on the PET website. A CD–ROM of training material has also been prepared, as noted in Section VIII.

The CEWES MSRC PET academic team accumulated a total of 472 person–days on–site at CEWES MSRC during Year 2, in addition to the permanent on–site personnel, divided among the support areas as follows:

Leadership (Mississippi State)	77 (Thompson)
CFD (Mississippi State)	101 (includes some SV and SPPT–MPI)
CSM (NCSA)	13
CWO (Ohio State)	38
EQM (Texas)	40
FMS & C/C (Syracuse)	23
C/C (NCSA)	15
SPPT (Rice/Tennessee)	70
SV (NCSA)	56
SV & C/C (JSU)	23
CSM & SV (CAU)	16

The team logged 80 person–days at remote user sites, and 22 person–days at Jackson State. The team had 101 person–days at the MSRC–wide Users Meeting, and 21 person–days at MSRC–wide PET meetings. There were 113 person–days at SC'97, and 114 person–days at other conferences, much of both being shared with the ASC and ARL MSRC PET efforts, where CEWES MSRC users were contacted and technology developments were presented and tracked.

Specific outreach activities conducted in Year 2 are described in this section, which is organized by individual components of the CEWES MSRC PET effort. And two major workshops related to outreach to users are described: a MSRC–wide Workshop with DoD CTA Leaders and a Cross–CTA Gridding Workshop.

But first there follows a summary of the CEWES MSRC User Taxonomy, which is continually updated in the course of the CEWES MSRC PET effort, in order to understand the makeup and potential needs of the CEWES MSRC user community.

CEWES MSRC User Taxonomy (97–01, 35)

The CEWES MSRC PET team first published a taxonomy of CEWES MSRC users in March 1997. At that time user statistics were only available for the Cray YMP and C90. Since then the YMP has been taken out of service, and utilization statistics have become available for the Cray T3E and IBM SP. A second taxonomy report is being prepared to analyze usage of the Cray C90 and T3E and the IBM SP. Some of the preliminary findings of that report are summarized here.

A comparison of Cray C90 utilization for July through December of 1997 with the same period in 1996 appears in the following table. The metric used in this comparison is Megaword–Hours, the product of memory words and CPU hours, and the Cray C90 utilization is presented in thousands of Megaword–Hours by CTA.

	CSM	CFD	SIP	CCM	CWO	CEA	EQM	Other
Jul–Dec 96	1,700	1,560	545	372	110	68	62	110
Jul–Dec 97	234	1,499	0.7	120	108	17	54	101

This illustrates a dramatic shift of HPC work to the new parallel platforms during the first half of 1997, due to a large extent by the migration of CSM work.

The previous taxonomy used Megaword–Hours as measure of resource utilization, which is appropriate for a vector computer with a global memory. However, it is less appropriate as a measure of utilization for parallel platforms where the amount of memory used is a function of the number of processors requested and may not be the actual amount of memory needed by the application. Thus, CPU–Hours is the utilization metric for the IBM SP and Cray T3E. The following table shows the utilization of these machines for September through November of 1997 in thousands of CPU hours by CTAs.

	CSM	CFD	SIP	CCM	CWO	CEA	EQM	CEN	FMS	Other
T3E Usage	202	54	6.1	47	102	9.3	–	7.1	–	8.8
SP Usage	59	39	3.3	29	94	–	1.2	–	4	5.2

From these results it is seen that the CSM and CWO users have been most active in utilizing these scalable parallel platforms.

The first user taxonomy showed a large percent of the CEWES MSRC users were not located on–site at CEWES. That continues to be true. The following table contains a list of the Cray C90 user locations using at least 5% of total C90 resources for July – December 1997 as indicated by account IDs. This may not indicate a user's physical location in all cases, however, since most of the users with accounts through ARO and ONR are located at universities.

C90

Institution	% Total MWH
AFRL–WPAFB	13.1
NRL–DC	12.5

NSWC–Carderock	10.9
CEWES	9.5
ONR–DC	7.9
ARL–Aberdeen	7.4
DSWA	7.4
AFOSR	6.7
AF Space & Missiles	5.6
AFRL–Kirtland	5.3

Similar statistics on locations of T3E and SP users are contained in the following two tables. These tables also contain the average number of processor elements used at each location. The results show that the users are taking advantage of the parallel processing capabilities of the T3E and SP.

T3E

Institution	Avg # PEs	% Total CPU
CEWES	75	48.3
NRL–Stennis	50	23.5
ONR–DC	73	10.9
AFRL–Edwards	62	10.9

SP

Institution	Avg # PEs	% Total CPU
NRL–Stennis	65	41.1
CEWES	34	28.3
ONR–DC	21	10.3
ARO	51	7.9

CFD: Computational Fluid Dynamics CTA

Interactions with CEWES MSRC users have been initiated by a variety of means. Telephone, email, and personal visits have all resulted in opportunities for CEWES MSRC user support and more specific collaborative efforts. Face–to–face visits have resulted from meeting DoD users at technical conferences such as the AIAA CFD meeting and annual AIAA Aerospace Sciences meeting.

Specific CEWES MSRC user outreach efforts have also been made. For example, In August 1997 a trip was made to AF Phillips Laboratory at Kirtland AFB. During this trip, we met with members of the Satellite Assessment Center. This trip has resulted in an ongoing collaboration with CEWES MSRC user David Medina of Phillips Lab (see the CFD part of Section V). User outreach has also been accomplished through the Parallel Programming Workshops wherein users are introduced to parallel programming within the context of their own code. This is a particularly effective opportunity for user outreach and training since it gives the on–site CTA lead an opportunity to meet and interact with users on an individual basis and learn about their work within a semi–formal classroom environment. Training conducted at remote user sites at DoD labs presents excellent opportunities for interacting with other CEWES MSRC users within our CTA.

Finally, both Bova and Thompson visited with Jay Boris, the DoD CTA Leader, on several occasions, and both Thompson and Bova had phone and email communication with Boris.

CSM: Computational Structural Mechanics CTA

The focus of the on–site user outreach in Year 2 was identifying the key on–site CSM CEWES MSRC users and determining their short–term and long–term requirements. Several meetings were held with Raju Namburu regarding his DoD Challenge Project work. Discussions were held with Robert Hall regarding the requirements of his Structural Analysis group and possible areas of CEWES MSRC PET support. The on–site lead (Weed) participated in meetings with Leon Chandler and Dave Medina at AF Phillips Lab regarding the CEWES MSRC PET effort. Meetings were held with Steve Akers of the CEWES Structures Lab to outline his work with the EPIC code and potential areas of CEWES MSRC PET support. Support was given to Larry Lynch in the Pavement Modeling group at CEWES to assist with his decision on funding university development of a parallel finite element solver.

LeRay Dandy and Bruce Loftis of NCSA visited Raju Namburu to discuss monitoring large CTH simulations during execution on a high performance computer and to discuss linking CTH and Dyna3D simulations. LeRay Dandy and Bruce Loftis visited Steve Akers to discuss simplifying EPIC analysis input. A Dyna3D–to–EPIC Translator has been developed to accomplish this task. LeRay Dandy and Bruce Loftis met with Steve Akers in regard to improving EPIC performance. EPIC runs on the Cray C90 which will be decommissioned during Year 3. LeRay Dandy met with Jon Windham and Doug Strasburg to discuss a new material model for CTH. Experimental work has been performed, and we have verified that current analytical models are inadequate.

CWO: Climate/Weather/Ocean Modeling CTA

OSU personnel Bedford, Sadayappan, Welsh, and Zhang visited CEWES MSRC to meet with CEWES MSRC user Bob Jensen and CWO on–site lead Cox. Discussions took place concerning the requirements for a seamless restart capability for the parallel WAM wave model. Further discussion concerned the requirements and strategies for the coupling of the WAM model, the CH3D marine circulation model, the COSED marine bottom boundary layer model, and the MM5 atmospheric circulation model.

Welsh and Jensen collaborated concerning how to add unsteady current and depth effects to WAM. It was concluded that the WAM pre–processor routines which pre–calculate the relevant arrays should be reused in the main calculation module, being called every time updated currents and depths are received from CH3D. Zhang and Billy Johnson exchanged emails concerning how to generate the grid mesh for Lake Michigan and verify the computation of temperature field with the current version of sequential CH3D code.

OSU personnel Bedford, Zhang, and O’Neil attended the 5th International Conference on Estuarine and Coastal Modeling at Alexandria, Virginia. They talked with experts in the field of Lake Michigan hydrodynamic modeling (e.g., David Schwab and Dmitry Belestkey of NOAA GLERL). They also discussed the problems of applying CH3D to Lake Michigan with Harry Wang.

Welsh and Jensen discussed the physical meaning of “wave stress” and “total stress” in the Janssen air/water boundary layer model in WAM. It was concluded that the wave stress should be used to modify the surface drag coefficient used in CH3D.

OSU personnel Bedford, Sadayappan, and Welsh met with Jensen, Christine Cuicchi of CEWES and Beaty of Cray/SGI at CEWES MSRC regarding the evaluation of the ongoing sequential and parallel WAM deployments on the various CEWES MSRC platforms. A Hurricane Luis simulation was selected for use and detailed plans were agreed on for deployment verification. The tests chosen focused on seamless restart and measurement of the differences between calculations made on the different platforms and with varying numbers of processors. Welsh met with Jensen to discuss the further verification of the pre–existing WAM current–induced propagation and refraction algorithms.

Welsh collaborated with Richard Strelitz, the CEWES MSRC PET SV on–site lead, concerning the use of OSU WAM and CH3D results for a visualization presentation. Welsh and Zhang subsequently provided Strelitz with the requested data plus sample extraction and plotting codes, sample plots and animations, and documentation of all materials.

EQM: Environmental Quality Modeling CTA

The TICAM team met with Jeff Holland numerous times to prioritize our efforts to meet DOD’s computational needs in this area. It was decided that environmental modeling in Cheseapeake and Florida bays was to be the number one project. This effort has involved weekly interactions with several members of the Mark Dortch’s (leader) group, Carl Cerco, Mark Noel, Barry Bunch and Ross Hall on the parallel migration of CE–QUAL–ICM. Through our joint efforts this parallel version is now in production mode. In addition, mesh partitioning software based on space filling curves was provided to this group. (This software was also given to Steve Bova, CFD CTA–on site).

Other EQM collaborations have involved providing code and training on the parallel hydrodynaamics code ADCIRC to Rao Vemulokanda and Norm Scheffner. The parallel migration of ADCIRC was completed at UTAustin.

Other interactions have involved discussions of groundwater, in particular solvers, discretization techniques and domain decomposition algorithms, with Joe Schmidt. There has also been discussions on how to improve the scalability of FEMWATER, an unsaturated flow code used by the hydrology community, with Fred Tracy.

FMS: Forces Modeling and Simulation/C4I CTA

As noted earlier, the natural HPCC user base in the DoD FMS community is not large. Consequently, the primary interface with the DoD FMS community has been through the DoD FMS CTA Lead, Robert Wasilausky of NRaD, and the various researchers involved in FMS CHSSI projects. In addition to routine contacts by email and at various meetings, Syracuse University’s FMS Lead, Wojtek Furmanski, was invited to attend an internal review of the FMS CHSSI program. This meeting, conducted at the Space and Naval Warfare Systems Command (SPAWAR) in San Diego, provided an opportunity for the CEWES MSRC PET team to keep abreast of CHSSI activities and for both groups to exchange views as to the evolution of the field.

During a visit to the Army Research Lab in Aberdeen MD, Furmanski also had the opportunity to talk with the heads of the Aberdeen Test Center and the Virtual Proving Ground project. Although these organizations are technically more closely allied with the IMT CTA area than with FMS, there is a fair amount of overlap between the two fields, especially in the opportunity for commodity distributed computing.

In conjunction with the CMS (Comprehensive Mine Simulator) parallelization planning effort, the Syracuse team has also had extensive contact with the code's owner, Steve Bishop, and his group at the Army Night Vision Lab at Ft. Belvoir. This included a visit by Furmanski to Ft. Belvoir for a briefing and demonstration of the system.

SPPT: Scalable Parallel Programming Tools

The primary source of CEWES MSRC user contact by the SPP Tools team members for the CEWES MSRC has been through workshops and courses:

- **"Parallel Tools and Libraries" workshop, held in April 1997 at Arnold Engineering Development Center (AEDC) by Christian Halloy (University of Tennessee), had 18 participants.**
- **"Parallel Tools and Libraries" workshop, held in July 1997 at CEWES MSRC by Susan Blackford (University of Tennessee) and Victor Eijkhout (UCLA), had 10 participants.**
- **"Performance Evaluation of Parallel Systems" workshop, held in July 1998 at CEWES MSRC by Erich Strohmaier (University of Tennessee), had 7 participants.**
- **"Workshop on Portable Parallel Performance Tools," held in January 1998 at CEWES MSRC by Shirley Browne (University of Tennessee) and Clay Breshears (Rice University), had 8 participants.**
- **"Code Optimization for MPPs" workshop, held in February 1998 at CEWES MSRC by Phil Mucci and Kevin London (University of Tennessee), had 12 participants.**
- **"Parallel Programming Workshop" held at the Naval Research Lab, Washington DC in March 1998 by the CEWES MSRC Computational Migration Group (CMG) and Breshears had 3 participants. There were three participants that received instruction on methods of parallelizing codes and tools available to help with such efforts.**

Clay Breshears, the on–site SPP Tools Lead, has consulted and collaborated with other on–site CTA Leads (Steve Bova, Rick Weed, Carey Cox) on tools and computer science issues. Breshears has also worked with Phil Bording, Jay Cliburn, Henry Gabb, Dan Nagle and Doug Strasburg of the CEWES MSRC Computational Migration Group (CMG) on code migration projects and the creation of CMG in–house conversion tools. The most notable collaboration has been the development and implementation of Fortran 90 bindings for POSIX threads on the SGI Origin 2000 at CEWES MSRC in support of the parallelization of the MAGI code (David Medina of the AF Phillips Lab) by the CMG. The at–Rice group (Ehtesham Hayder, Chuck Koelbel, Gina Goff) met with CMG members Strasburg, Bording, Gabb at CEWES MSRC to discuss use of parallel tools in code migration related to HELIX and MAGI codes. Hayder also contacted David Medina and Ted Carney (New Mexico Tech) about the MAGI code.

Shirley Browne, of Tennessee, and Breshears have worked with CMG members in the use of parallel performance analysis tools. Use of these tools has provided CMG members another method of approaching their code migration efforts and measuring the efficiency of codes that have been parallelized. Browne and Breshears also worked with members of the VPRF DoD Challenge Project group from Kirtland AFB when they visited CEWES MSRC in March 1998, and using VAMPIR they were able to improve the communication performance of the ICEPIC code.

Jack Dongarra, Clint Whaley, and Antoine Petitet corresponded with CEWES MSRC user Alan Wallcraft (NRL–Stennis) about the possibility of using ScaLAPACK for the ocean modeling DoD Challenge Project in June and July 1997. David O'Neal (PSC) visited CEWES MSRC and worked with Breshears and Cox on writing a matrix inversion code using ScaLAPACK routines on the SGI/Cray T3E at CEWES MSRC. This code is used as a preprocessing step to the Wallcraft ocean model code. Blackford and Whaley were consulted for advice on correctness of the implementation.

Breshears has worked with Brian Jean and Alan Stagg (CEWES MSRC application engineers) and Joe Schmidt (CEWES Coastal Hydraulics Laboratory) on the design and creation of SPLICE (Scalable Programming Library for Coupling Executables). This will be a high–level library to allow separate MPI codes (possibly running on separate HPC platforms) to trade information with each other. SPLICE is intended to give researchers the ability to couple diverse codes without having to be concerned with minute details of data layout and distribution within each code.

SV: Scientific Visualization

As part of a long–term collaboration, the CEWES MSRC PET Scientific Visualization team has had ongoing communication with Carl Cerco and Mark Noel of CEWES, in relation to their Chesapeake Bay project and visual analysis of the output of the CEWES CE–QUAL–IQM code. This is a continuation of the relationship that was begun in Year 1. During Year 2, we have worked with them on defining their requirements for desktop visualization support, prototyping solutions for those needs, and iterating on the design process to refine their specifications. We have provided them an early version of a tool that they are currently using to view data from their 10– and 20–year production runs of the Chesapeake Bay model. This tool also supports a limited form of collaboration that they are using to share their results with their project monitor at the Environmental Protection Agency.

We have also begun a significant collaboration with CSM users Raju Namburu, Tommy Bevins, Byron Armstrong, and Photios Papados, in relation to their DoD Challenge Project in simulation of damaged structures. In support of their effort, we have provided a tool to view the results of both their CTH and Dyna3D simulations. This tool allowed them to verify the results of these runs, particularly the Dyna3D output. It has also allowed them to generate visualizations in the form of static images and mpeg movies to share with their colleagues over the Web. We also used this tool to highlight and explain their science at the national meeting, SC97.

C/C: Collaboration/Communication

NCSA hosted the first MSRC PET Webmasters Meeting Feb 3 – 5, 1998. Attendees included both PET and MSRC webmasters from the CEWES, ASC, ARL, and NAVO MSRCs. The objectives of the meeting were 1) to build a sense of community among the MSRC/PET webmasters to facilitate communication and sharing and 2) to identify mechanisms to improve usability and uniformity across the MSRC PET websites. The meeting resulted in a list of suggestions for presentation to the PET directors at the MSRCs for their approval. These suggestions have been incorporated into ongoing C/C core support plans.

MSRC–wide Workshop with DoD CTA Leaders

In September 1997, the CEWES MSRC PET team participated in a MSRC–wide workshop between the DoD CTA Leaders and the leadership of the CTA support teams in the PET effort at all four MSRCs. Prior to this workshop, the DoD CTA Leaders had prepared White Papers for each CTA citing MSRC user needs that might be addressed in the PET effort at the MSRCs. After this workshop, the PET academic leadership prepared responses to these White Papers. And out of this workshop came the impetus for the PET roadmaps and vision statements organizing future directions of the PET effort in five essential areas:

- **Metasystems**
- **Programming Tools**
- **Application Tools**
- **Scientific Visualization**
- **Training & Collaboration**

These documents are available from the CEWES MSRC PET website.

Cross–CTA Gridding Workshop

As a part of the CEWES MSRC PET Year 2 effort, a workshop on the utility of grid generation systems for MSRC users was held at the University of Texas in Austin in February 1998 (see the last part of Section V). This grid workshop was targeted specifically at five “grid–related” CTAs: CFD, CSM, CWO, EQM, and CEA. This grid workshop served both to identify the needs of CTA users that are not being met with currently available grid (mesh) generation systems, and to broaden the awareness of the availability of grid generation resources in the CEWES MSRC user community (see Section VII).

X. HBCU/MI ENHANCEMENT PROGRAM

For Year 2 of the PET component of the DoD HPCMP, the Historically Black Colleges and Universities/Minority Institutions (HBCU/MI) team consisted of Jackson State University (JSU), Central State University (CSU), and Clark Atlanta University (CAU). JSU, located in Jackson, MS, is the lead HBCU/MI at the CEWES MSRC. CSU, located in Wilberforce, Ohio, is the lead for the ASC MSRC, while Clark Atlanta University (CAU), located in Atlanta, Georgia, is the lead at the ARL MSRC. While each university plays the major role at its home MSRC, with respect to the HBCU/MI program, each institution is also committed to making technical contributions to the PET effort, and to the overall HPC modernization effort.

This section describes how these institutions participated in PET initiatives at the CEWES MSRC during the second year of the program, and how the institutions were enhanced by their involvement. Training courses and seminars conducted by the CEWES MSRC PET team at HBCU/MIs are listed in Table 8.

Five training courses or seminars were conducted at the HBCU/MI member sites of the CEWES MSRC PET team: four at Jackson State and one at Clark Atlanta, impacting over 170 students and faculty from these and three other HBCUs.

As the lead university at the CEWES MSRC, JSU is charged with developing and implementing strategies that allow a two–way exchange between the DoD and HBCU/MI communities. On the one hand, minorities are tremendously underrepresented in the Computational Technology Areas (CTAs) and other HPC efforts within the DoD. On the other hand, the existing pool of talent available to address current and future DoD challenges, using HPC technologies, is limited. The PET program provides the DoD with an opportunity to identify and develop new sources of scientific, high–tech, and management personnel. In the opposite direction, PET affords faculty, staff, and students, at HBCU/MIs, an opportunity to acquire scientific and HPC–related skills and expertise through interaction with DoD scientists and researchers. JSU's mission is to maximize mutual benefit for both sides by helping to create and maintain pathways between the CEWES MSRC and the HBCU/MI team. Adequate access to HPC machinery, and other information technology resources, is critical to HBCU/MI participation in this endeavor.

1. Facilities at JSU

During Year 2, JSU made substantial upgrades to its computing and networking facilities through the CEWES MSRC PET program. In addition, JSU faculty members were able to collaborate with colleagues at major research universities, as well as with DoD scientists, researchers, and engineers. Three new staff members were hired and participated in training activities at both JSU and the CEWES MSRC. Students (a list of students impacted by the CEWES MSRC PET effort is given in Table 9) were the ultimate beneficiaries, receiving direct access to a state–of–the–art learning environment and curriculum enhancement. Students from JSU and other HBCU/MIs attended the 1997 Introductory HPC Summer Institute, sponsored by the CEWES MSRC, while JSU students received new course offerings.

2. Web–Based Distance Education at JSU

In collaboration with the Northeast Parallel Architectures Center (NPAC) at Syracuse University in the CEWES MSRC PET effort, JSU held Web–Based Distance Education courses during the Fall

1997 and Spring 1998 semesters. Computer Science students, physically located at JSU, were taught "Programming for the Web" by instructors located at Syracuse University. The classroom was equipped, through the CEWES MSRC PET program, with sixteen personal computers, ergonomic furniture, and a T–1 line connection to the DREN through the CEWES MSRC. Mike Robinson was hired as JSU's Network Training Specialist, to set up and support the classroom hardware and software. This included configuring the T–1 router, coordinating and setting Internet addresses for the computers, and installing/maintaining NPAC's Tango/WebWisdom collaborative software. Robinson received training at both NPAC and the CEWES MSRC. In addition, two JSU Computer Science Assistant Professors, Drs Debasis Mitra and Qutaibah Malluhi, participated in the class as on–site instructors. The classroom equipment, along with the experience gained by the JSU personnel, will allow JSU to deliver training to CEWES MSRC users over the Web. JSU is also now in a position to set up distance learning classrooms at other HBCU/MIs and deliver courses to them.

3. Scientific Visualization at JSU

JSU also participated in scientific visualization support at the CEWES MSRC during Year 2 in training and experimentation. Two areas of focus included 1) training JSU faculty, staff, and students, in addition to CEWES MSRC users and, 2) in partnership with the National Center for Supercomputer Applications (NCSA) at the University of Illinois, developing techniques for doing remote scientific visualization. Through the CEWES MSRC PET program, JSU was able to equip a "Sci Viz" lab with five high end graphics workstations, all connected to the DREN through the CEWES MSRC T–1 line. Mildred "Milti" Leonard and Edgar Powell were hired to provide hardware and software support, as well as to assist with training. Milti worked closely with the University of Illinois scientific visualization team during a three–month extended visit to NCSA in the Fall of 1997. Both Milti and Edgar maintained constant contact and interaction with the CEWES MSRC and administered workshops at JSU. Dr Gwang Jung, a JSU Associate Professor of Computer Science, worked closely with the PET group, while Dr Mitra did preliminary development of a semester–long course. The scientific visualization equipment and personnel enhancements at JSU have placed the University in an excellent position to increase support to the CEWES MSRC and to other HBCU/MIs.

4. Other HBCU/MIs

Although an attempt is made to coordinate the HBCU/MI effort across the entire PET program, different universities assume lead roles at the individual MSRCs, as described above. Therefore, major enhancements at CSU and CAU were accomplished through the ASC and ARL MSRCs, respectively.

As a member of the HBCU/MI team, CSU was an early collaborator in the Web–Based Distance Education project. Through this collaboration, CSU's ability to receive courses from other institutions was significantly enhanced. In addition, CSU students were eligible to attend the HPC Summer Institute held at JSU.

During Year 2, CAU participated in PET at the CEWES MSRC through a focused effort titled "Residual Capacity and Damage Assessment Evaluation and Visualization ." This project allowed close collaboration between CAU faculty, staff, and students, and CEWES MSRC personnel. CAU's distance education and scientific visualization capabilities were enhanced greatly by involvement with JSU and the CEWES MSRC. CAU students were also invited to participate in JSU's HPC Summer Institute.

CEWES MSRC PET TECHNICAL REPORTS

The following is a list of CEWES MSRC PET Technical Reports that have been produced in Year 2. The items with numbers have completed the review process and are ready for distribution to CEWES MSRC users.

1. 97–01 S.W. Bova, C.W. Mastin, and C. Cox, **"A Taxonomy of Major CTA Software at CEWES MSRC,"** CEWES MSRC/PET TR/97–01, Vicksburg, MS, May 1997.

   Abstract: The subject of this study is the set of applications categorized under the CFD, CSM, CWO, and EQM CTA's which was run on the Cray C916 and YMP at the CEWES MSRC during the last six months of 1996. These particular CTA's were chosen because they have on–site specialists to provide support for CEWES users. The objectives are to identify the users who consume the most computational resources, determine basic features of their software, and obtain a flavor of their associated physical applications.

2. 97–02 S.W. Bova, **"Some Performance Issues Associated with CEWES MSRC Scalable Architectures,"** CEWES MSRC/PET TR/97–02, Vicksburg, MS, December 1997.

   Abstract: Some typical performance issues associated with sparse matrix codes which use the Message Passing Interface and distributed memory machines will be discussed. In particular, average, sustained, floating point performance will be examined as a function of problem size and number of processors for an unstructured fluid mechanics solver. These issues will be examined within the context of the iterative solution of nonsymmetric, linear systems of equations, such as those that arise from finite volume approximations to convection–diffusion problems. A brief description of the parallel CGSTAB (stabilized bi–conjugate gradient) iterative method will be followed by comparisons of its performance on the IBM SP, SGI Origin 2000, and Cray T3E at the CEWES MSRC. In general, these machines have chips that are rated at several hundred Mflops, but actual performance obtained in practice is much less. Sustained performance is a strong function of cache and communication performance. The aim of this report is not to determine which machine is ''better'' for certain classes of problems, but rather to illustrate performance trade–offs that users can expect to address in most problems run on these machines.

3. 98–01 C.W. Mastin, **"1997 CEWES MSRC PET Training Activities,"** CEWES MSRC/PET TR/98–01, Vicksburg, MS, January 1998.

   Abstract: Training is the most visible part of the PET program for many of the CEWES MSRC users. During 1997, the PET training program passed several milestones. The first large conference, the Colloquium on HPC Collaborative Methods and Tools, was held at CEWES in February before an audience of approximately 100 DoD users from across the country. The first remote training class was also held in February, and now remote classes have become a routine part of our training schedule. Service to remote users was also improved when classes moved to the the Training and Education Facility (TEF). The TEF is furnished with professional quality video production and recording equipment. This has enhanced the Mbone broadcasts and improved the quality of recorded classes in the tape library. This report contains a list of all training activities during the 1997 calendar year.

4. 98–02 S. Browne, J. Dongarra and K. London, **“Review of Performance Analysis Tools for MPI Parallel Programs,”** CEWES MSRC/PET TR/98–02, Vicksburg, MS, March 1998.

   Abstract: For this review, we have investigated a number of performance tools, both research and commercial, that are available for monitoring and/or analyzing the performance of MPI message–passing parallel programs written in Fortran or C. We investigated the following tools:

   AIMS–instrumentors, monitoring library, and analysis tools; MPE logging library and nupshot performance visualization tool; Pablo–monitoring library and analysis tools; Paradyn–dynamic instrumentation and run–time analysis tool; SvPablo–integrated instrumentor, monitoring library, and analysis tool; VAMPIR trace monitoring library and VAMPIR performance visualization tool; VT–monitoring library and performance analysis and visualization tool for the IBM SP.

   The most prevalent approach taken by these tools is to collect performance data during program execution and then provide post–mortem analysis and analysis display of performance information. The exception to this from the above list is Paradyn, which provides interactive run–time analysis. To give our review continuity and focus, we followed a similar procedure for testing each tool and used a common set of evaluation criteria.

5. 98–03 S.W. Bova, **“A Fortran90 Module for Message–Passing Applications with Unstructured Communication Patterns,”** CEWES MSRC/PET TR/98–03, Vicksburg, MS, January 1998.

   Abstract: For high–performance scientific computing, message–passing is often the paradigm of choice: MPI, the Message–Passing Interface standard. Incorporating a message–passing capability within an application involves the consideration of several bookkeeping issues such as the number and identity of processors with which a given processor communicates and the identification of data which must be exchanged. Many computational mechanics applications have unstructured communication patterns so that simply representing the data associated with a message is a cumbersome task. If the application is written in C or C++, the use of structures or classes provides a natural way to organize this data. However, the majority of scientific applications are written in Fortran. This work describes one way in which this data can be organized within a Fortran program which uses a finite element method to solve a partial differential equation. This approach exploits some of the new features of Fortran90. Since Fortran77 is a subset of Fortran90, existing Fortran77 codes can easily use the proposed approach by switching to a Fortran90 compiler and incrementally adding the new language features (e.g. modules, dynamic memory allocation, global variables, and user–defined datatypes). Moreover, the data structures are bundled with functions in the spirit of a C++ class.

6. 98–04 C.P. Breshears, **“Survey of the Construction and Utility of PET Virtual Workshops,”** CEWES MSRC/PET TR/98–04, Vicksburg, MS, January 1998.

   Abstract: Cornell Theory Center (CTC) provided a Virtual Workshop on “Parallel Computing and Programming Languages” that was sponsored by the DOD HPC Modernization Program. This workshop was held over the World Wide Web with participants able to download course materials and make use of the IBM SP from the CTC.

Since the CTC Virtual Workshop is a possible remote training environment, this workshop was monitored to judge the effectiveness of virtual workshops for presentation of PET training materials.

7. 98–05 S.W. Bova and C.P. Breshears, **“Using the MPE Graphics Library with Fortran90,”** CEWES MSRC/PET TR/98–05, Vicksburg, MS, February 1998.

   Abstract: The MPE graphics library is part of the MPICH package distributed by Argonne National Laboratory. This graphics library gives the MPI programmer an easy–to–use, minimal set of routines that can asynchronously draw color graphics to an X11 window during the course of a numerical simulation. Unfortunately, there is little scientific visualization software written for MPE, which places a high burden on the applications programmer. This difficulty is compounded by a dearth of documentation on the library. On the other hand, the library is small and has a shallow learning curve. This report is a brief description of how these graphics routines may be called from a Fortran90 program, written from the perspective of a finite element applications programmer. It was written after gaining one week of experience in the use of the MPE graphics library, thereby demonstrating that the library is compact enough to be easily used if the applications programmer is familiar with graphics programming. A goal of this report is to make the package equally useful to those programmers who are not as familiar with graphics programming.

8. 98–06 **“Contract Year Two Programming Environment and Training (PET) Additional Focused Efforts for CEWES Major Shared Resource Center (MSRC),”** CEWES MSRC/PET TR/98–06, Vicksburg, MS, February 1998.

   Abstract: As a result of the Mid–Year Review for the U.S. Army Corps of Engineers Waterways Experiment Station (CEWES) Major Shared Resource Center (MSRC) Programming Environment and Training (PET) program that occurred on 22–23 September 1997, additional Focused Efforts were approved for the primary Computational Technology Areas (CTAs) supported by the center and for other specialty areas.

9. 98–07 J. Zhu, P. Bangalore, D.H. Huddleston and A. Skjellum, **“On the Parallelization of CH3D,”** CEWES MSRC/PET TR/98–07, Vicksburg, MS, March 1998.

   Abstract: CH3D (Curvilinear Hydrodynamics in 3–Dimensions) is a hydraulic simulation code that has been used to model various coastal and estuarine phenomena. It is a complex, legacy code with more than 18,000 lines. The code is capable of handling highly irregular geometric domains involving coastal, estuarine, and riverine environments. It has been used by the U.S. Army Corps of Engineers for both purely hydrodynamic simulations and as a foundation for many of the environmental quality modeling and sediment transport models. As such, the reduction of execution time of CH3D is critical to various DoD hydrodynamics simulations and environment quality modeling projects.

   For historical reasons, there has been a large number of production codes written in Forran for vector computers. The data structure, controlling logic, and the numerical algorithms in these codes are in general not suitable for parallel computers. The parallelization work on CH3D not only reduces the execution time for this code, but also provides valuable experience on porting other complex application codes with similar data structures and numerical schemes from vector computers to parallel computers, thereby generating a significant impact on the computer simulation work in the DoD user community.

This report summarizes the work on parallelizing the CH3D code. It covers basic mathematical models, numerical algorithms used in the code, parallelization strategies, code modifications, numerical experiments, and recommendations for further efficiency improvement.

10. 98–08 S. Browne, J. Dongarra, J. Horner, P. McMahan and S. Wells, **"Software Repository Interoperation and Access Control,"** CEWES MSRC/PET TR 98–08, Vicksburg, MS, March 1998.

    Abstract: With funding from the ARL, ASC, and CEWES MSRCs, the Repository in a Box (RIB) toolkit produced by the National High–performance Software Exchange (NHSE) project is being used to set up a network of interoperable DOD CTA software repositories. This paper discusses repository interoperation and access control issues relevant to this effort.

11. 98–09 C.O.E. Burg, D.H. Huddleston and R.C. Berger, **"A Computational Design Method for High–Velocity Channels,"** CEWES MSRC/PET TR/98–09, Vicksburg, MS, March 1998.

    Abstract: With the growth of urban centers in recent years and the resulting changes in infrastructure, the capacity of many existing storm water management systems has been stretched to its limit. Altered surface hydrology increases surface runoff which reaches drainage channels more quickly, resulting in greater system loads. To handle this increased flow, many of these channels need to be redesigned. Complicating this process are the restrictions on channel designs due to other structures, such as roads, bridges and multi–story buildings, because alterations to these structures can be quite expensive. Designing high–velocity channels to handle the increased water flow while minimizing the alterations to existing structures is a formidable task, with the current design technique being a trial and error approach.

    In this paper, we present an efficient, deterministic design method, which applies the adjoint variable formulation of direct differentiation to a computational, open–channel flow model in order to obtain the derivative of an objective function with respect to the design variables. From these derivatives, we modify the design variables with the goal of minimizing the objective function. The particular CFD code (HIVEL2D) uses an unstructured, Petrov–Galerkin, finite element method to solve the unsteady, two–dimensional, depth–averaged, shallow water equations. The test cases involve channel contraction problems with one, two and three design variables, where uniform downstream flow is the goal. For these cases, the iterative design process produces channels that yield about a 90% improvement over straight wall contractions.

12. 98–10 S. Chippada, C. Dawson, V.J. Parr, M.F. Wheeler, C. Cerco, B. Bunch and M. Noel, **"PCE–QUAL–ICM: A Parallel Water Quality Model Based on CE–QUAL–ICM,"** CEWES MSRC/PET TR/98–10, Vicksburg, MS, March 1998.

    Abstract: CE–QUAL–ICM is a three–dimensional eutrophication model developed at the U.S. Army Corps of Engineers Waterways Experiment Station (CEWES), Vicksburg, MS. This water quality model is semi–explicit in time, and is based on an unstructured cell–centered finite volume numerical method. The hydrodynamics data such as velocities and turbulent diffusion are read in externally, and the model computes the advection–diffusion–reaction of a number of physical and state variables such as temperature, salinity, sediments, oxygen, algae, etc. This sequential FORTRAN 77 code was parallelized using data/domain decomposition strategy and a single program, multiple data (SPMD) paradigm. WQMPP, a pre/post–processor for the water quality model which splits the global domain into a specified number of smaller subdomains and sets up the local data files and message passing tables, has been developed. WQMPP, when run in post–processor mode also combines the local subdomain output to produce global output in a format similar to that produced by the original CE–QUAL–ICM code. PCE–QUAL–ICM, the parallel water quality model enhances CE–QUAL–ICM with message passing. Inter–processor communication is done using MPI communication libraries and the parallel code has been ported onto the CRAY–T3E, IBM–SP2 and SGI O2000. This paper explains the domain decomposition and parallelization strategy employed in WQMPP and PCE–QUAL–ICM.

13. 98–11 M.F. Wheeler, C. Dawson, S. Chippada, M. Martinez and V.J. Parr, **"Progress Report: Parallelization of ADCIRC3D,"** CEWES MSRC/PET TR/98–11, Vicksburg, MS, March 1998.

    Abstract: This report summarizes recent work on the parallelization of the ADCIRC shallow water simulator. ADCIRC is a finite element model developed by Luettich and Westerink, and is used at CEWES for modeling of bays and estuaries. The parallelization effort involves an SPMD approach, whereby a preprocessing code partitions the mesh, and partitions global input datasets among the processors. The code is modified to include MPI message passing calls to handle the transfer of data among processors. A postprocessing code was developed to take the local output from each processor and reassemble global output files. Two mesh partitioning strategies are discussed, one based on the node ordering as given by the mesh generator, and one based on a space–filling curve reordering of the mesh. It is seen by numerical experiments that the space–filling curve approach is superior.

14. 98–12 M.P. Baker and E.L. Peters, **"Comparing Middleware Support Systems for Collaborative Visualization,"** CEWES MSRC/PET TR/98–12, Vicksburg, MS, March 1998.

    Abstract: Habanero and Tango are two freely available pacakages designed to support the development of collaborative applications. We experimentated with using these middleware support systems to enable collaborative use of an existing tool for three–dimensional visual data analysis. In each case, migrating our application presented challenges, but was ultimately successful. Here we report on that experience and compare and contrast these two middleware support systems in terms of their ability to support our application.

15. 98–13 Lex Lane, Frank Baker and Sandie Kappes, **"netWorkPlace Project Report,"** CEWES MSRC/PET TR/98–13, Vicksburg, MS, March 1998.

    Abstract: The netWorkPlace (nWP) implementation for the CEWES MSRC site demonstrated an early investigative use of online collaboration technology in support of a set of researchers and support staff teams. The approach was to implement an application suite developed and used at NCSA, and promote its use at CEWES MSRC for a variety of collaboration and administrative processes and teams. After approximately one year of use, an analysis of the nWP environment was performed to evaluate its successes and shortcomings, further refine the collaboration requirements of the teams that did and might employ such tools, and drive a decision process on further tool suite implementations. This document looks at the early history of nWP development at NCSA, why it was chosen for early implementation and evaluation at the CEWES MSRC site, the results of the analysis of its actual use, and the implications and recommendations for further customization and tool suites for collaboration.

16. 98–14 D. Welsh, S. Zhang, P. Sadayappan and K. Bedford, **"WAM Performance Improvement and NLOM Optimization,"** CEWES MSRC/PET TR/98–14, Vicksburg, MS, March 1998.

    Abstract: This report summarizes work during Year 2 of the PET CWO Core Support effort at CEWES MSRC. The activities included training, user outreach, challenge support, parallel migration support, and parallel algorithm/tools development. Significant effort was placed on parallel migration support and parallel algorithm development, especially in optimization and enhancement of the parallel WAM (WAve Model) code, a workhorse code for CWO and a code needed in a CWO focused effort project on coupling wave, circulation and sedimentation models.

17. 98–15 S. Zhang, D. Welsh, P. Sadayappan, K. Bedford, and S. O'Neil, **"Coupling of Circulation, Wave and Sediment Models,"** CEWES MSRC/PET TR/98–15, Vicksburg, MS, March 1998.

    Abstract: Implementation and computational testing of the coupled circulation, wave and sediment codes (CH3D, WAM and CH3D–SED) was done using Lake Michigan as the modeling domain. Both one–way and two–way couplings were made between WAM and CH3D. The dynamical effects of wave–current interactions at the surface are reported for demonstration examples.

18. 98–16 M.P. Baker, D. Bock, R. Heiland and M. Stephens, **"Visualization of Damaged Structures,"** CEWES MSRC/PET TR/98–16, Vicksburg, MS, March 1998.

    Abstract: This report summarizes our experience in providing visualization support for a study of blast propagation from a car bomb and structural damage to a neighboring building. In this study, CTH was used to simulate the bomb blast. Dyna3D was used to model the building's structural response to the pressure loadings from the bomb blast. The visualization done for this study included examination of slice planes and isosurfaces for the bomb blast, as well as modeling the building deformation over time.

19. 98–17 R. Machiraju, Z. Zhu, B. Fry and R. Moorhead, **"Structure Significant Representation of Structured Datasets,"** CEWES MSRC/PET TR/98–17, Vicksburg, MS, March 1998.

    Abstract: Numerical simulation of physical phenomena is now an accepted way of scientific inquiry. However, the field is still evolving with a profusion of new solution and grid generation techniques being continuously proposed. Concurrent and retrospective visualization are being used to validate the results, compare them among themselves and with experimental data, and browse through large scientific databases. There exists a need for representation schemes which allow access of structures in an increasing order of smoothness (or decreasing order of significance). We describe our methods on datasets obtained from curvilinear grids. Our target application required visualization of a computational simulation performed on a very remote supercomputer. Since no grid adaptation was performed, it was not deemed necessary to simplify or compress the grid. In essence, we treat the solution as if it were in the computational domain. Inherent to the identification of significant structures is determining the location of the scale coherent structures and assigning saliency values to them. Scale coherent structures are obtained as the result of combining across scales the coefficients of a wavelet transform. The result of this operation is a correlation mask that delineates regions containing significant structures. A spatial subdivision (e.g., octree) is used to delineate regions of interest. The mask values in these subdivided regions are used as a measure of information content. Later, another wavelet transform is conducted within each subdivided region and the coefficients are sorted based on a perceptual function with bandpass characteristics. This allows for ranking of structures based on the order of significance, giving rise to an adaptive and embedded representation scheme. We demonstrate our methods on two datasets from computational field simulations. Essentially we show how our methods allow the ranked access of significant structures. We also compare our adaptive representation scheme with a fixed blocksize scheme.

20. 98–18 J.E. West and R. Machiraju, **“A Numerical Imaging Approach to Comparative Visualization,”** CEWES MSRC/PET TR/98–18, Vicksburg, MS, March 1998.

Abstract: Numerical simulation is now an acceptable mode of inquiry into a wide range of physical phenomena. As computational methods and hardware continue to advance, it is often the case that older, legacy applications no longer implement the best technology for solving a problem and must be updated. Once modified, these applications need to be extensively studied to ensure that they retain the important characteristics of the original application (accuracy, convergence, etc.). Furthermore, as experimental techniques continue to advance, it is possible to extensively validate existing numerical simulation applications with more accurate physical measurements. Side–by–side comparison and juxtaposition facilitate visual verification of verisimilitude. However in many applications the datasets are too large and complex, and visualization techniques too complex or poorly–understood, to rely solely on visual verification. In the present work a quantitative, computable metric is proposed which incorporates both quantitative measures and a visual comparison element to highlight the differences between two datasets. The comparison metric is multipart and captures the spatial spread of the differences, and can also highlight the differences in regions of high and low transitions.The metric can be applied to both datasets and images alike. We demonstrate the effectiveness of the proposed metric on a variety of examples. These proposed methods can not only be used for examples from the computational sciences, but can also be applied towards the comparison of datasets and images from other domains including medical.

21. 98–19 S. Chippada, C.N. Dawson, M.L. Martinez and M.F. Wheeler, **“A Projection Method for Constructing a Mass Conservative Velocity Field,”** CEWES MSRC/PET TR/98–19, Vicksburg, MS, March 1998.

Abstract: In the numerical modeling of fluid flow and transport problems, frequently the velocity field needs to be projected from one finite dimensional space into another. In certain applications, especially those involving modeling of multi–species transport, the new projected velocity field should be accurate as well as locally mass conservative.

In this paper, a velocity projection method has been developed that is both accurate and mass conservative element–by–element on the projected grid. The velocity correction is expressed as gradient of a scalar pressure field, and the resultant Poisson equation is solved

using a mixed/hybrid finite element method and lowest–order Raviart Thomas spaces. The conservative projection method is applied to the system of shallow water equations and a theoretical error estimate is derived.

22. 98–20 G.C. Fox, W. Furmanski and H.T. Ozdemir, **"JWORB – Java Web Objects Request Broker for Commodity Software Based Visual Dataflow Metacomputing Programming Environment,"** CEWES MSRC/PET TR/98–20, Vicksburg, MS, March 1998.

Abstract: Programming environments and tools that are simultaneously sustainable, highly functional, robust and easy to use have been hard to come by in the HPDC area. This is partially due to the difficulty in developing sophisticated customized systems for what is a relatively small part of the worldwide computing enterprise. As the commodity software becomes naturally distributed with the onset of Web and Intranets, we observe now a new trend in the HPDC community to base high performance computing on the modern enterprise computing technologies.

This approach was not possible still a few years ago when: a) the enterprise computing was still mainly custom TP Monitors based client–server (2–tier) only; and b) Web computational extensions such as CGI were too naive to grant high performance and/or quality of service. However, the ongoing covergence of Web and Enterprise Computing accelerates the development of scalable (multi–server) and open 3–tier standards such as CORBA, DCOM or Enterprise JavaBeans and our vision becomes quickly a reality these days. We can now start prototyping both user friendly and powerful HPDC systems by merging the commodity technologies in tier 1 (front–end) and tier 2 (application logic) with the high performance technologies in tier 3 (legacy software).

Initial Web/Commodity based HPDC prototypes appeared in the pure Java domain. We summarize here our experience with one such early system, WebFlow for visual dataflow metacomputing developed at NPAC in '96/'97. Basically, we found Java to be a very useful framework for middleware development whereas both front–end and back–end development require both multi–platform and multi–language support – which led us in a natural way to the CORBA model. We are now building and reporting here on the current status of our new CORBA based WebFlow with the middleware/bus layer given by a mesh of Java Web Object Request Brokers (JWORB).

23. 98–21 E. Akarsu, G.C. Fox, W. Furmanski, T. Haupt, H. Ozdemir, Z. Odcikin Ozdemir and T. Pulikal, **"Building Web/Commodity based Visual Authoring Environments for Distributed Object/Component Applications – A Case Study using NPAC WebFlow System,"** CEWES MSRC/PET TR/98–21, Vicksburg, MS, February 1998.

Abstract: We present here an approach towards visual authoring environments for Web/Commodity based distributed object/componentware computing using the WebFlow system under development at NPAC as a case study. WebFlow is a 3–tier Java–based visual dataflow system with applets–based authoring, visualization and control front–ends, and with servlets–based middleware management of backend modules that wrap legacy codes such as databases or high performance simulations. We summarize here the WebFlow architecture; we describe a set of demos and early applications in various areas of distributed computing (including imaging, collaboration, condensed matter physics and military wargaming simulations); and we outline the next phase design, based on lessons learned in

the current prototype. New WebFlow uses JWORB (Java Web Object Request Broker) middleware and employs WOMA (Web Object Management Architecture) methodology to establish a testbed for testing, evaluating and integrating the emergent componentware standards of CORBA, DCOM, Java and W3C/WOM.

24. 98–22 D. Dias, G.C. Fox, W. Furmanski, V. Mehra, B. Natarajan, H. Timucin Ozdemir, Shrideep Pallickara and Zeynep Ozdemir, **"Exploring JSDA, CORBA and HLA based MuTech's for Scalable Televirtual (TVR) Environments,"** CEWES MSRC/PET TR/98–22, Vicksburg, MS, February 1998.

    Abstract: We discuss here new distributed computing technologies of relevance for building multi–user scalable televirtual (TVR) environments on the Internet such as: Java Shared Data API (JSDA) by JavaSoft, Common Object Request Broker Architecture (CORBA) by Object Management Group (OMG) and High Level Architecture (HLA) by Defense Modeling and Simulation Office (DMSO). We describe our early TVR prototype based on VRML2 front–end and JSDA back–end, and we summarize our ongoing work on exploring CORBA Events and HLA Dynamic Data Distribution technologies for building scalable collaboration servers for the Internet.

25. 98–23 G.C. Fox, W. Furmanski, B. Natarajan, H. T. Ozdemir, Z. Odcikin Ozdemir, S. Pallickara and T. Pulikal, **"Integrating Web, Desktop, Enterprise and Military Simulation Technologies to Enable World–Wide Scalable Televirtual (TVR) Environments,"** CEWES MSRC/PET TR/98–23, Vicksburg, MS, February 1998.

    Abstract: We present an approach to the next generation televirtual (TVR) environments that integrate collaboration with distributed computing and modern modeling and simulation technologies. We follow the 3–tier architecture with the Web Object (Java/CORBA) based middleware, VRML/Java3D/DirectX based front–ends and JDBC/PSS/OLEDB based backends and we are testing our design and the integration concepts by prototyping a multi–user authoring and runtime environment to support WebHLA based distributed military simulations. We present first our taxonomy of collaboratory frameworks and our integration paradigm, based on the WebFlow system at NPAC. We then list the critical enabling technologies that are being integrated and finally we summarize the current status of our prototyping experiments.

26. 98–24 M.P. Baker, **"VisGen Cross–Platform Visualization,"** CEWES MSRC/PET TR/98–24, Vicksburg, MS, March 1998.

    Abstract: In this focused effort, we are developing strategies that will allow us to build visualization tools for both the desktop and virtual reality display systems. We have taken care to encapsulate the functionality involved in mapping data to graphic form. This visualization–generator capability is then coupled with various user interfaces and used in various settings. To date, we have used our visualization generator in a desktop tool, and a Web–based VRML–server tool. We are working towards incorporation in an ImmersaDesk tool. In this setting, the VisGen code will be coupled with a multimodal interface, utilizing speech and gesture at the interface, and augmenting the visualization with non–speech audio.

27. 98–25 P.J. Mucci and K. London, **"The CacheBench Report,"** CEWES MSRC/PET TR/98–25, Vicksburg, MS, March 1998.

    Abstract: CacheBench is a benchmark designed to evaluate the performance of the memory hierarchy of computer systems. Its specific focus is to parameterize the performance of possibly multiple levels of cache present on and off the processor. This paper describes CacheBench and presents benchmark results on the CEWES MSRC Cray T3E, IBM SP, and SGI Origin 2000.

28. 98–26 P.J. Mucci and K. London, **"The MPBench Report,"** CEWES MSRC/PET TR/98–26,Vicksburg, MS, March 1998.

    Abstract: MPBench is a benchmark to evaluate the performance of MPI and PVM on MPPs and clusters of workstations. MPBench currently tests six different message–passing metrics or calls: send bandwidth, send roundtrip, send application latency, broadcast, reduce, and allreduce. This paper describes MPBench and presents results on the CEWES MSRC Cray T3E, IBM SP, and SGI Origin 2000.

29. 98–27 P. J. Mucci and K. London, **"The BLASBench Report,"** CEWES MSRC/PET TR/98–27, Vicksburg, MS, March 1998.

    Abstract: BLASBench is a benchmark designed to evaluate the performance of some kernel operations of different implementations of the BLAS routines. The BLAS are the Basic Linear Algebra Subroutines and are found in some form or another on most vendors' machines. BLASBench currently benchmarks the three most common routines in the BLAS. They are: AXPY: Vector addition with scale GEMV: Matrix–Vector multiplication with scale GEMM: Matrix–Matrix multiplication with scale. This paper describes BLASBench and presents results on the CEWES MSRC Cray T3E, IBM SP, and SGI Origin 2000.

30. 98–28 B. Jean, R. Weed and J.F. Thompson, **"Grid Generation Capabilities Enhancement at the CEWES MSRC,"** CEWES MSRC/PET TR/98–28, Vicksburg, MS, April 1998.

    Abstract: It is recognized that no one grid tool will solve all the grid generation problems faced by users in the various CTAs. It is also recognized that the strengths and weaknesses of the different existing commercial and public domain grid generation systems and their suitability for application in the user's specific CTA are not known to the user community. Therefore, tools that might reduce a particular user's grid generation time are not being used because the user is unaware of their existence. Also, many users have specific enhancements they would like to see in existing tools. Because of the importance of the grid generation process in computational simulations and the need to address the specific grid generation needs of the CEWES MSRC users, a Focused Effort was initiated under the CEWES MSRC Programming, Environment, and Training (PET) program to first evaluate existing commercial and public domain grid generation software and then use the information gained from the evaluations and from interactions with users to define a strategy for enhancing the grid generation capabilities for the both users of the CEWES MSRC and the DoD in general. This white paper describes the work performed to obtain and evaluate a wide variety of commercial and public domain grid generation software that represent the currently available state of the art in grid generation.

31. 98–29 T. Scavo, D.E. Bernholdt, G.C. Fox, R.Markowski, N.J. McCracken, M. Podgorny and D. Mitra, **"Synchronous Learning at a Distance: Experiences with Tango,"** CEWES MSRC/PET TR/98–29, Vicksburg, MS.

    Abstract: In the fall of 1997, the Northeast Parallel Architectures Center at Syracuse University taught a computational science course at Jackson State University in Jackson, Mississippi, using the Tango collaboratory system. What made this course unique is that twice a week instructors “met” with students online, showing lecture slides and programming examples, and discussing concepts in real time over the Internet. The goal of the project was to investigate the use of Tango in teaching a traditional lecture–based course in a distance–learning format.

32. 98–30 L.C. Burton, R. Machiraju and D.S. Reese, **“Identifying Boundary Anomalies to Facilitate Correct Parallel Image Composition,”** CEWES MSRC/PET TR/98–30, Vicksburg, MS, March 1998.

    Abstract: Parallel image composition presents an attractive approach to run–time visualization of structured grid data. However, certain configurations of grid boundaries prevent composition from being performed correctly. In particular, when the boundary between two partitions contains concave sections, the partitions may no longer be depth sorted correctly, a requirement for some visualiza tion techniques such as raycasting. If the data may be repartitioned such that it can be depth sorted correctly, then an image composition approach is a viable option. To facilitate such an operation, we present an algorithm to analyze the geometric structure of a grid boundary and extract knowledge about how the boundary impacts depth sorting and therefore image composition.

Submitted and awaiting final edits/final corrections

33. 98–31 L.S. Hebert, W.G. Seefeld and A. Skjellum, **“MPICH on the Cray T3E,”** CEWES MSRC/PET Technical Report, Vicksburg, MS.

    Abstract: The authors describe their efforts to support the ubiquitous MPI programming model, based on the MPICH 1.1 implementation, on the the Cray T3E. Discussion of porting issues, performance issues, and protocol decisions are offered. Future work opportunities and challenges are also reported.

34. 98–32 C.P. Breshears, H.A. Gabb and S.W. Bova, **“Towards a Fortran90 Interface to the POSIX Threads Library,”** CEWES MSRC/PET Technical Report, Vicksburg, MS.

35. 98–33 L.S. Blackford and R.C. Whaley, **“ScaLAPACK Evaluation and Performance at the DoD MSRCs,”** CEWES MSRC/PET Technical Report, Vicksburg, MS.

    Abstract: ScaLAPACK is a library of high–performance linear algebra routines for distributed–memory message–passing MIMD computers and networks of workstations supporting PVM and/or MPI. This paper presents performance results for a subset of the ScaLAPACK driver routines and PBLAS routines on the Cray T3E, IBM SP, SGI Origin 2000, and SGI Power Challenge Array platforms at CEWES MSRC.

36. 98–34 D. Bernholdt, G.C. Fox, W. Furmanski, B. Natarajan, J.T. Ozdemir, Z. Odcikin Ozdemir and T. Pulikai, **“WebHLA – An Interactive Programming and Training Environment for High Performance Modeling and Simulation,”** CEWES MSRC/PET Technical Report, Vicksburg, MS.

37. 98–35 R.H. Pritchard and H. Moore, **“Update to Taxonomy of Major Computation Technology Area (CTA) Software at CEWES Major Shared Resource Center (MSRC),”** CEWES MSRC/PET Technical Report, Vicksburg, MS.

38. 98–36 O. Olatidoye, S. Sarathy, G. Jones, L. Milligan and C. McIntyre, **“A Representaive Survey of Blast Loading Models and Damage Assessment for Buildings Subject to Explosive Blasts,”** CEWES MSRC/PET Technical Report, Vicksburg, MS.

Abstract: This effort was focused primarily on determining the state of the art in the area of blast loading models and damage assessment methods for buildings subject to explosive blasts. The effort consisted of a literature search of representative articles dealing with analysis and prediction of blast effects on buildings as a result of terrorist acts. Much work in the area of blast analysis has been done prior to this, however, a majority of this information is still restricted due to its military significance. In addition to actual blast loading due to explosions, a small selection of articles related to impact loading, as in the case of a earthquakes, was also reviewed. The search was conducted in two broad thrusts: first the articles on blast load modeling were identified. While there were several hundred relevant articles on this subject, the actual mathematical formulation used to describe the transient pressure loading of a building in the vicinity of a external explosion did not vary a great deal. The second thrust was in identifying damage assessment methods used to characterize failure and damage in the context of blast loaded structures. The majority of articles reviewed used some combination of material constitutive relationships and bounds on the static or dynamic structural deformation to identify and in some cases quantify damage. In most part, there was very little distinction between degraded load capacity, impending failure and damage. Very few of these approaches, in their present form, will be helpful for the purposes of visualization and decision support.

39. 98–38 H.A. Gabb, R. P. Bording, S.W. Bova and C.P. Breshears, **"A Fortran90 Application Programming Interface to the POSIX Treads Library,"** CEWES MSRC/PET Technical Report, Vicksburg, MS.

40. 98–39 Gina Goff, C. Koelbel, B. Robey and D. Torres, **"Performance Evaluation of HPF Kernels on the IBM SP and CRAY T3E,"** CEWES MSRC/PET Technical Report, Vicksburg, MS.

Abstract: We have executed several small tests representative of the sorts of operations commonly found in scientific applications on the SP and T3E at CEWES MSRC, in an effort to provide DoD users with guidelines as to which approaches are likely to work best. The tests are written in HPF, a data–parallel Fortran language available on both computers and fall into three basic categories: communication kernels, intrinsics, and computational kernels. Multiple variants of many computations were tested, to see if undertaking an operation in a certain way had a significant impact on performance. Speedup for 4, 16, and 64 processors was measured by dividing the iterations per second for multiple processors by the number of iterations per second for the uniprocessor case. We also compared the number of iterations/second for the serial version on the same number of processors. The "uniprocessor" type of speedup indicates how well a particular test scales, while the "serial version" speedup is meant to show how effective a given optimization is. In general, communications were expensive, especially reduction, although serial version speedups were usually quite respectable. Intrinsics also had unimpressive uniprocessor–type speedup, but showed excellent serial version speedups that increased with the number of processors, most notably when array syntax or REDISTRIBUTE was used. By comparing speedups, we found that programs that scale well on one test machine will probably have acceptable if not optimal behavior on the other. We also found a significant amount of overlap on each machine between the test variations with good uniprocessor–type speedup and the ones having good serial–version speedup, indicating that variants that scale well also tend to be good optimizations.

41. Contract Year Three Programming Environment and Training (PET) Core Support and Focused Efforts for CEWES Major Shared Resource Center (MSRC).

42. G.E. Fagg and K.S. London, **"MPI Interconnection and Control,"** CEWES MSRC/PET Technical Report, Vicksburg, MS.

Abstract: The main goal of the MPI–Connect project is to allow different MPP vendor MPI implementations to intercommunicate to allow the use of multiple MPPs in solving challenge problems. Intercommunication allows users to place each section of an application on the system most suited for its execution. Targeted users of MPI–Connect are those who have such multi–platform applications and those who need dynamic process control and cannot wait for MPI–2 to appear. This paper describes technical issues in porting the MPI–Connect system to CEWES MSRC platforms, in particular the Cray T3E. Also described are the anticipated uses of MPI–Connect for FMS and CWO applications.

43. R.C. Whaley and J. Dongarra, **"Automatically Tuned Linear Algebra Software,"** CEWES MSRC/PET Technical Report, Vicksburg, MS.

Abstract: ATLAS is an approach for the automatic generation and optimization of numerical software for processors with deep memory hierarchies and pipelined functional units. The production of such software for machines ranging from desktop workstations to embedded processors can be a tedious and time consuming task. ATLAS has been designed to automate much of this process. Initial efforts have concentrated on the widely used linear algebra kernels called the Basic Linear Algebra Subroutines (BLAS). This paper discusses the ATLAS approach, gives timing comparisons for ATLAS–generated BLAS with vendor BLAS on DOD MSRC platforms, and discusses the relevance of ATLAS for the DOD MSRCs.

44. Y. Zhu and D.E. Bernholdt, **"CEWES Database Projects Developed by NPAC,"** CEWES MSRC/PET Technical Report, Vicksburg, MS.

Abstract: This report summarizes two Focused Efforts with a common theme of coupling commercial database technology with the world–wide web to facilitate the presentation and management of large information spaces. The two project titles are "Web–Linked Databases for Domain–Specific Information Repositories" and "Interfacing Databases and the Web: Management of Large WWW Sites Using Commercial Database Technology." Both projects utilize the Oracle7 relational database system, the Oracle Context Option and the Oracle Web Server. The services provided can be accessed using any standard web browser.

45. R. Machiraju, Z. Zhu, B. Fry and R. Moorhead, **"Structure Significant Representation of Computational Field Simulation Datasets,"** CEWES MSRC/PET Technical Report, Vicksburg, MS.

Abstract: Numerical simulation of physical phenomena is now an accepted way of scientific inquiry. However, the field is still evolving with a profusion of new solution and grid generation techniques being continuously proposed. Concurrent and retrospective visualization are being used to validate the results, compare them among themselves and with experimental data, and browse through large scientific databases. There exists a need for representation schemes which allow access of structures in an increasing order of smoothness (or decreasing order of significance). We describe our methods on datasets obtained from curvilinear grids. Our target application required visualization of a computational simulation performed

on a very remote supercomputer. Since no grid adaptation was performed, it was not deemed necessary to simplify or compress the grid. In essence, we treat the solution as if it were in computational domain. Inherent to the identification of significant structures is determining the location of the scale coherent structures and assigning saliency values to them. Scale coherent structures are obtained as a result of combining across scales the coefficients of a vavelet transform. The result of this operation is a correlation mask that delineates regions containing significant structures. A spatial subdivision (e.g., octree) is used to delineate regions of interest. The mask values in these subdivided regions are used as a measure of information content. Later, another wavelet transform is conducted within each subdivided region and the coefficients are sorted based on a perceptual function with bandpass characteristics. This allows for ranking of structures based on the order of significance, giving rise to an adaptive and embedded representation scheme. We demonstrate our methods on two datasets from computational field simulations. Essentially we show how our methods allow the ranked access of significant structures. We also compare our adaptive representation scheme with a fixed blocksize scheme.

JOURNAL PAPERS & CONFERENCE PRESENTATIONS
Related to Year 2 CEWES MSRC PET Effort

CFD: Computational Fluid Dynamics CTA

1. J. Zhu, B. Johnson, P. Bangalore, D.H. Huddleston and A. Skjellum, **"A Portable and Scalable Three–Dimensional Hydrodynamic Simulator for Parallel Computers,"** *SC97,* San Jose, CA, November 1997.

   Abstract: We will discuss the development of a parallel version of a three–dimensional, hydraulic simulation code (CH3D) which has been used to model various coastal and estuarine phenomena. This is a complex, legacy code with more than 18,000 lines. The code is capable of handling highly irregular geometric domains involving coastal lines and rivers and has been widely used by US Army Corps of Engineers for hydrodynamic and water quality modeling. This is a collaborative project between US Army Engineer Waterways Experiment Station and Mississippi State University, and the effort is conducted under the auspices of the new DOD High Performance Computing Modernization Program. The parallel implementation is based on domain decomposition. The linear solver is based on an ADI–type algorithm which is parallelized using a wavefront approach. Interprocessor communication is handled using MPI, making the parallel code portable to a wide range of multiprocessor computers. The major challenge is to deal with complicated data structure involved in real simulation problems with irregular geometries and interprocessor communications for data exchange. Timing results obtained on the SGI PCA/Origin and Cray T3E for simulating the New York Bay will be presented to demonstrate significant reduction of the execution time using multiprocessors.

2. D.H. Huddleston, R.C. Berger and C.O.E. Burg, **"A Computational Design Method for High–Velocity Channels,"** *Mississippi Section American Society of Civil Engineers Spring '97 Meeting,* Vicksburg, MS, April 1997. ***(Presentation Only, No Abstract)***

3. J. Zhu, P. Bangalore, D.H. Huddleston and A. Skjellum, **"On the Development of a Parallel Three–Dimensional, Hydrodynamic Simulator,"** *1998 ASCE International Water Resources Engineering Conference,* Memphis, TN, August 1998.

   Abstract: CH3D (Curvilinear Hydrodynamics in 3–Dimensions) is a hydraulic simulation code that has been used to model various coastal and estuarine phenomena. It is a complex, legacy code with more than 18,000 lines. The code is capable of handling highly irregular geometric domains. It has been used by the US Army Corps of Engineers for both purely hydrodynamic simulations and as a foundation for many of the environmental quality modeling and sediment transport models. This paper summarizes the work on parallelizing the CH3D code. It covers basic mathematical models, numerical algorithms, parallelization strategies, code modifications, and numerical experiments.

4. C.O.E. Burg, D.H. Huddleston and R.C. Berger, **"A Numerical Design Method for Open–Channel Flow,"** *1998 ASCE International Water Resources Engineering Conference,* Memphis, TN, August 1998.

   Abstract: With the growth of urban centers and the resulting changes in infrastructure, the capacity of many existing storm water management system has been stretched to its limit. Altered surface hydrology increases surface runoff which reaches drainage channels more quickly, resulting in

greater system loads. to handle this increased flow, many of these channels need to be redesigned. Complicating this process are the restrictions on channel designs due to other structures, such as roads, bridges and buildings, because alteratins to these structures can be expensive. Designing high–velocity channels to handle the increased water flow while minimizing the alteratins to existing structures is a formidable task, with the current design technique being a trial and error approach. In this paper, we present an efficient, deterministic design method, which applies the adjoint variable formulation of direct differentiation to a computational, open–channel flow model (HIVEL2D) in order to obtain the derivative of an objective function with respect to the design variables. From these derivatives, the design variables are modified with the goal of minimizing the objective function. The test cases involve channel contraction problems with one, two and three design variables.

5. S.W. Bova, **"Parallel Solution of a Streamline Upwind Petrov–Galerkin Model of the Shallow Water,"** Poster Session, *SC'97,* San Jose, CA, November 1997.

   Abstract: This poster will discuss the parallel performance of a streamline upwind Petrov–Galerkin finite element approximation to the two–dimensional, depth–averaged shallow water equations. Time–iterative solutions are obtained using enhanced stability, multi–stage Runge–Kutta methods on unstructured triangular grids. The implementation is in Fortran 90 and performs asynchronous message passing using MPI. Fortran 90 facilitates the implementation of the unstructured communication patterns through its allowance of user–defined data types that can be bundled with functions in a module. Results are computed for a portion of the upper Mississippi river using the distributed memory computers at the Department of Defense's CEWES Major Shared Resource Center.

6. Z. Wanxie, X. Zhuang and J. Zhu, **"A Self–Adaptive Time Integration Algorithm for Solving Partial Differential Equations,"** *Applied Mathematics and Computation,* Vol. 89, 1997, 295–312.

   Abstract: Non–uniform spatial grids are commonly used to resolve locally fast–changing physical phenomena in space. If a traditional explicit time integration scheme is used to advance solutions in the temporal dimension, the step size is restricted by the stability criterion, which is in turn dictated by the smallest grid spacing in the spatial dimensions. It turns out that the excessively small time step enforced by the smallest spatial grid spacing in a domain is usually unnecessary for most of the grid points with larger grid spacing. A new adaptive time integration method is introduced in this paper to improve the computational efficiency. The basic idea is to use different time step sizes at different spatial grid points. The stability criterion is still satisfied at all grid points by using different time step sizes. In this way, the time step size adjusts automatically based on the local spatial grid spacing. Complexity analysis and implementation details are also discussed in the paper. The non–linear Burger's equation is used in the numerical experiment. Both the complexity analysis and numerical computations demonstrate significant improvement of computational efficiency.

CSM: Computational Structural Mechanics CTA

1. O. Olatidoye, S. Sarathy, G. Jones, C. McIntyre, L. Milligan and R. Namburru, **"Scientific Visualization for Interpretation and Assessment of Damage in Structures Subject to Blast Loads,"** Submitted to the *DoD HPC Users Group Conference,* Houston, TX, June 1998.

   Abstract: There has been significant activity in computational structural mechanics community, in developing methods to identify, assess and predict the effects of explosive blast loading on structures. The use of high performance computing tools in analysis and prediction of blast loading has provided an unprecedented insight and understanding on the mechanisms of failure, as well as methods to assess this damage in these cases. However, these analyses produce vast amounts of data, which are difficult to visualize. Researchers at Clark Atlanta University in collaboration with CEWES MSRC have developed a basic testbed to validate different visualization paradigms associated with different damage rules specifically for the visualization of blast analysis data. This paper outlines this framework and describes the approach adopted.

CWO: Climate/Weather/Ocean Modeling CTA

1. D. Welsh, S. Zhang, P. Sadayappan, K. Bedford, and S. O'Neil, **"Coupling of Marine Circulation and Wave Models,"** Submitted to the *DoD HPC Users Group Conference*, Houston, TX, June 1998.

Abstract: Marine circulation and wind–wave calculations have traditionally been made separately, but in recent years the potential importance of interactions between the two motions has been recognized. In shallow water and high current regions in particular, the interactions can be very large. There has been coupled model research in the past decade, but simplified models have generally been used and the full power of high performance computers has not been applied. One focused effort of the CEWES MSRC PET Climate, Weather, and Oceanography (CWO) program has therefore been to couple advanced circulation and wave models in a robust, flexible, and physically realistic manner, taking full advantage of the CEWES MSRC facilities. The CH3D circulation model and the WAM wave model are being used in this project. Both codes contain advanced physics and are already used in sequential form at CEWES MSRC. The CH3D model predicts three–dimensional current, temperature, and salinity fields, plus the two–dimensional water surface elevation field; standard inputs are wind speeds, surface heat fluxes, and tributary inflows. The model uses a mode–splitting technique in which the baroclinic, internal motions and barotropic, external motions are solved for separately and combined in a consistent manner. A terrain–following sigma coordinate system is used in the vertical dimension, with a regular curvilinear grid in the horizontal. The WAM model (cycle 4) is based on the conservation of action density on a regular spherical grid for a two–dimensional frequency–direction spectrum of components. All significant shallow water effects are included, with source/sink terms for wind input, nonlinear wave–wave interaction, whitecapping, and bottom friction. The basic version can accommodate a steady current field. The field is input in the pre–processing stage and the resulting current propagation and refraction effects are held constant for the duration of the simulation. Wind fields at regular intervals are a required input. Nested gridding is an available option. Lake Michigan was chosen as the computational domain for the prototype coupling of CH3D and WAM. This selection simplifies the specification of accurate boundary conditions, and the lake is also the site of the NOAA EEGLE project, an ongoing, extensive data collection program. A 3 minutes longitude by 2 minutes latitude grid (approximately 4 km square cells) was re–sampled from high density bathymetry data; both models use this grid. The reliability of the basic CH3D Lake Michigan deployment was confirmed by the reproduction of classical Kelvin wave behavior, including coastal upwelling. Similarly, WAM was found to correctly predict standard fetch–limited wave growth. To achieve model coupling, CH3D has been modified to accept radiation stress and wave stress (which modifies surface roughness) from WAM, giving altered surface momentum inputs in the barotropic mode. WAM has been modified to use unsteady currents and unsteady depths. The WAM source/sink term algorithms have also been reformulated to reflect the modulation of wave frequencies by currents. A user–specified coupling frequency has been implemented. An idealized test case has been used to evaluate the realism and impact of the various couplings. In the idealized test, a 10

m/s North wind is applied for 30 hours, followed by a 6 hour rotation, then a 10 m/s West wind for 30 hours. Results have been compared for no coupling, one–way coupling (models run separately, writing to file, then re–run, reading the other model's arrays from file), and two–way importance of particular mechanisms. In CH3D, radiation stress effects were small, but wave stress effects led to storm surge increases of up to 70% and current modulations up to 100%. In WAM, current propagation and refraction effects caused 5% increases in maximum lake wide significant wave height; unsteady depths caused negligible differences. The impact of the modulated source/sink terms has not yet been evaluated, but it is expected that the reduction of wave height due to modified wind input will dominate the current propagation and refraction effects. Details are provided on:

1. **Our experiences with the coupling of the WAM and CH3D codes**

2. **Our experiences with optimization of the codes on various CEWES MSRC platforms including the SGI Origin2000, IBM SP2 and Cray T3E.**

For example, unexpected sources of communication overhead were discovered in the first version of the parallel WAM code (which was developed as part of a previous CHSSI effort). Seemingly paradoxically, the introduction of additional inter–processor synchronization was able to significantly improve performance: Performance data for a 24 hour WAM simulation of Hurricane LUIS on the SGI Origin2000:

	5 PEs	**12 PEs**	**21 PEs**
Total time (old)	**14913**	**1931**	**3561**
Total time (new)	**8114**	**1286**	**2189**

We hope that the reporting of some of our experiences in optimizing the parallel codes may be of interest to other users of DoD HPCMP parallel machines.

2. Shuxia Zhang and Keith Bedford, **"Scaling Character and Prediction of Wave Energy Over a Multi–Dynamics Regime: Example of Lake Erie Field Experiment,"** Submitted to the *1998 Western Pacific Geophysics Meeting*, 1998.

Abstract: Multi–level analysis via wavelet transform has been performed for the temporal variations of wave energy, which is derived from the in situ water elevation data measured with high sampling rate in Lake Erie during a series of field experiments in 1996. The analysis objectives are two fold: one is to better understand the scale–to–scale variability of wave energy, especially under the storm winding condition, in the complicated hydrodynamical system of Great Lakes, which consists of multi–dynamical interactions among the turbulence, wave propagation, current circulation, sediment suspension, and more. The second is to investigate whether a predictive relationship exists in the intrinsic evolution of wave energy from one dynamical regime to another, which can be described with a simple mathematical (or statistical) formalism.

Two new findings are reported in this paper. The first one is that under strong wind conditions (speed > 10 knots) the standard deviations of wave energy fluctuations exhibit gaussianility and simple scaling (or fractal similarity) exists over the multi–dynamical regimes, whose characteristic time scale varies from several seconds (turbulence) to a few hours (storm–induced swell). The second one is that the magnitude of the scale invariant depends on the averaged wind kinetic energy. This dependence renders a link between the larger–scale wind forcing and the small–scale statistics of turbulence. Based on the two findings, a dynamic scheme is developed for predicting the wave energy and further the waveheights over multi–dynamical regimes overlapping in the Great Lakes.

Conditional on the wind energy being provided, this scheme can predict very well the wave energy variations down to the turbulence regime. Combined with numerical forecasting models, this scheme also provides a useful tool to predict the possible range of wave heights during severe weather.

EQM: Environmental Quality Modeling CTA

1. **"Finite Element Approximations to the System of Shallow Water Equations, Part II: Discrete Time A Priori Error Estimates,"** to appear in *SIAM Journal of Numerical Analysis*, 1998.

   Abstract: Various sophisticated finite element models for surface water flow exist in the literature. Gray, Kolar, Luettich, Lynch and Westerink have developed a hydrodynamic model based on the generalized wave continuity equation (GWCE) formulation, and have formulated a Galerkin finite element procedure based on combining the GWCE with the nonconservative momentum equations. Numerical experiments suggest that this method is robust, accurate and suppresses spurious oscillations which plague other models. In this paper, we analyze a closely related Galerkin method which uses the conservative momentum equations (CME). For this GWCE–CME system of equations, we present, for discrete time, an a priori error estimate based on an L2 projection.

2. S. Chippada, C. Dawson, M. Martinez and M.F. Wheeler, **"A Projection Method for Constructing A Mass Conservative Velocity Field,"** *Computer Methods in Applied Mechanics and Engineering,* Vol. 157, pp. 1–10, 1998.

   Abstract: In the numerical modeling of fluid flow and transport problems frequently the velocity field needs to be projected from one finite dimensional space into another. In certain applications, especially those involving modeling of multi–species transport, the new projected velocity field should be accurate as well as locally element–by–element mass conservative. In this paper, a velocity projection method has been developed that is both accurate and mass conservative cell–by–cell on the projected grid. The velocity correction is expressed as gradient of a scalar pressure field, and the resultant Poisson equation is solved using a mixed/hybrid finite element method and lowest–order Raviart Thomas spaces. The conservative projection method is applied to the system of shallow water equations and a theoretical error estimate is derived.

3. S. Chippada and C. Dawson, **"Numerical Modeling of Shallow Water Flows with Wetting and Drying Boundaries by a Finite Volume Method,"** *Proceedings of the Society for Computer Simulation Western Multiconference*, San Diego, CA, January 1998.

   Abstract: A finite volume method on unstructured meshes has been developed for solving the system of shallow water equations. The system of equations is formulated as a conservation law, and integrated over each cell. The solution is approximated on each cell by constants or linears. Numerical fluxes at cell interfaces are computed using Roe's approximate solution of the Riemann shock–tube problem. This paper outlines the method and discusses the extension of this procedure to physical problems involving wetting and drying.

SV: Scientific Visualization

1. R. Machiraju, Z. Zhu, B. Fry and R. Moorhead, **"Significant Representation of Structured Datasets,"** *IEEE Transactions of Visualization and Graphics,* Vol. 4, No 2, pp. 117–132, June 1998.

   Abstract: Numerical simulation of physical phenomena is now an accepted way of scientific inquiry. However, the field is still evolving with a profusion of new solution and grid generation techniques being continuously proposed. Concurrent and retrospective visualization are being used to validate the results, compare them among themselves and with experimental data, and browse through large scientific databases. There exists a need for representation schemes which allow access of structures in an increasing order of smoothness (or decreasing order of significance). We describe our methods on datasets obtained from curvilinear grids. Our target application required visualization of a computational simulation performed on a very remote supercomputer. Since no grid adaptation was performed, it was not deemed necessary to simplify or compress the grid. In essence, we treat the solution as if it were in the computational domain. Inherent to the identification of significant structures is determining the location of the scale coherent structures and assigning saliency values to them. Scale coherent structures are obtained as the result of combining across scales the coefficients of a wavelet transform. The result of this operation is a correlation mask that delineates regions containing significant structures. A spatial subdivision (e.g., octree) is used to delineate regions of interest. The mask values in these subdivided regions are used as a measure of information content. Later, another wavelet transform is conducted within each subdivided region and the coefficients are sorted based on a perceptual function with bandpass characteristics. This allows for ranking of structures based on the order of significance, giving rise to an adaptive and embedded representation scheme. We demonstrate our methods on two datasets from computational field simulations. Essentially we show how our methods allow the ranked access of significant structures. We also compare our adaptive representation scheme with a fixed blocksize scheme.

2. J.E. West and R. Machiraju, **“A Numerical Imaging Approach to Comparative Visualization,”** Submitted to *Visualization’98*, Research Triangle Park, NC, 1998.

   Abstract: Numerical simulation is now an acceptable mode of inquiry into a wide range of physical phenomena. As computational methods and hardware continue to advance, it is often the case that older, legacy applications no longer implement the best technology for solving a problem and must be updated. Once modified, these applications need to be extensively studied to ensure that they retain the important characteristics of the original application (accuracy, convergence, etc.). Furthermore, as experimental techniques continue to advance, it is possible to extensively validate existing numerical simulation applications with more accurate physical measurements. Side–by–side comparison and juxtaposition facilitate visual verification of verisimilitude. However in many applications the datasets are too large and complex, and visualization techniques too complex or poorly–understood, to rely solely on visual verification. In the present work a quantitative, computable metric is proposed which incorporates both quantitative measures and a visual comparison element to highlight the differences between two datasets. The comparison metric is multi–part and captures the spatial spread of the differences, and can also highlight the differences in regions of high and low transitions.The metric can be applied to both datasets and images alike. We demonstrate the effectiveness of the proposed metric on a variety of examples. These proposed methods can not only be used for examples from the computational sciences, but can also be applied towards the comparison of datasets and images from other domains including medical.

SPPT: Scalable Parallel Programming Tools

1. H. Gabb, P. Bording, S.W. Bova, C.P. Breshears and D. Medina, **“Expressing Fine–Grained Parallelism Using Fortran Bindings to Posix Threads,”** accepted for presentation in the *Fortieth Cray User Group Conference*, June 1998.

   Abstract: In dynamics simulations, the through–space interactions between particles, which must be calculated every time step, consume the bulk of computational time. These calculations typically occur in a single large loop containing many data dependencies. However, the iterations are often independent, so fine–grained parallelism should confer a significant performance gain. Pthreads have significant advantages over compiler directives, which often create separate UNIX processes. Multiple threads exist in a single process and require less system overhead. Also, threads are not linked to physical processors as is often the case for compiler directives. Multiple threads residing on a single processor give better resource utilization (e.g., separate threads doing computation and I/O operations). Performance and programming issues that arise when expressing fine–grained parallelism on SGI SMP and Cray T3E architectures will be discussed.

2. C. Breshears and S. Browne, **"Usability Study of Portable Parallel Performance Tools,"** Submitted to the *DoD HPC Users Group Conference*, Houston, TX, June 1998.

   Abstract: This paper describes a usability study of four trace–based parallel performance tools that are designed to be portable across parallel platforms: AIMS, nupshot (with MPE logging), SvPablo, and VAMPIR. The tools have been deployed at the University of Tennessee and at the DoD CEWES MSRC in Vicksburg, MS. Surveys, group walkthroughs, and field observations have been carried out to determine which features are most useful and why, and to make suggestions for improvements.

3. S. Blackford and C. Whaley, **"ScaLAPACK Evaluation and Performance at the DoD MSRCs,"** Submitted to the *DoD HPC Users Group Conference,* Houston, TX, June 1998.

   Abstract: ScaLAPACK is a library of high–performance linear algebra routines for distributed–memory message–passing MIMD computers and networks of workstations supporting PVM and/or MPI. This paper presents performance results for a subset of the ScaLAPACK driver routines and PBLAS routines on the Cray T3E, IBM SP, SGI Origin 2000, and SGI Power Challenge Array platforms at the CEWES, ARL, ASC, and NAVO Major Shared Resource Centers (MSRCs).

4. P. Mucci and K. London, **"Architecture Characterization of DoD MSRC HPC Platforms,"** Submitted to the *DoD HPC Users Group Conference*, Houston, TX, June 1998.

   Abstract: This paper presents performance results for a set of low–level architecture characterization benchmarks that collectively measure the dense numerical computation rate, bandwidth to multiple levels of the memory hierarchy, and the message passing performance of several high performance architectures. The architectures evaluated include the Cray T3E, IBM SP, and SGI Origin 2000 platforms at the CEWES, ARL, ASC, and NAVO Major Shared Resource Centers. The results should be of interest to application developers and systems planners as a point of reference for performance modeling and scalability analysis.

5. C.P. Breshears, H.A. Gabb and S.W. Bova, **"Towards a Fortran 90 Interface to the POSIX Threads Library,"** Submitted to the *DoD HPC Users Group Conference*, Houston, TX, June 1998.

   Abstract: Pthreads is a POSIX standard established to control the spawning, execution and termination of multiple threads within a single process. Use of Pthreads on a shared memory system is an attractive approach due in part to a low overhead. The disadvantage of Pthreads, with respect to high performance computing, is that there is no Fortran interface defined as part of the POSIX standard. To this end, we present our current progress in defining and implementing a full set of Fortran 90 bindings for the POSIX threads functions along with programming tricks used and lessons learned while striving to keep the bindings as portable as possible. Also, our investigation of combining Pthreads with MPI is described. This hybridization of two such diverse programming models is attractive for distributed clusters of SMP nodes.

6. S. Browne, G. Goff, C. Koelbel, P. Mucci and E. Strohmaier, **“Parallel Performance Evaluation and Modeling in the DoD Modernization Program,”** Poster Session at *SC’97*, San Jose, CA, November 1997.

   Abstract: Benchmarking and performance modeling form an important part of high performance computing practice. Within the DoD HPC Modernization Program, these topics are of interest for:

   - **Planning future hardware procurements**
   - **Evaluating current applications software**
   - **Developing and optimizing future applications software**
   - **Training users of parallel machines**

   We are addressing these needs through an integrated performance evaluation and performance modeling project. Performance evaluation is done using the PARKBENCH codes, a well–known set of public–domain benchmarks. We are extending the PARKBENCH low–level, kernel, and compact applications to include codes in High Performance Fortran, and to include examples representative of DoD applications. Our long–term goal is to use results from these benchmarks as inputs to performance models, which can in turn estimate performance of full applications. This poster will present our plans, and preliminary results from PARKBENCH codes on codes at the DoD Major Shared Resource Centers.

7. G. Goff, C. Koelbel, B. Robey and D. Torres, **“Performance Evaluation of HPF Kernels on the SP and T3E,”** Submitted to 1998 *DoD HPC Users Group Conference*, Houston, TX, June 1998.

   Abstract: Unfamiliarity with parallel languages and how their implementations are likely to behave can be a major obstacle for many users trying to migrate code to parallel machines. We have executed several small tests representative of the sorts of operations commonly found in scientific applications on the SP and T3E at CEWES MSRC. The tests are written in HPF and our intent is to provide general guidelines for CEWES MSRC users by showing them which approaches are likely to yield the best performance in the environments already at their disposal. The tests fall into three basic categories: communication kernels, intrinsics, and computational kernels. An important aspect of HPF is its promise of a “efficiently portable programming style”. That is, when there are several ways to express the same computation, the relative efficiencies of different variants should not vary wildly from machine to machine. We tested this aspect of HPF and found that programs that scale well on one of the machines often have acceptable if not optimal behavior on the other.

C/C: Collaboration/Communication

1. Press Release: **“Newly Emergent Web Technologies Make Unique Distance Learning Course a Reality,”** Syracuse University, 22 October 1997.

2. T.R. Scavo, M.Podgorny and N.J. McCracken, **“Synchronous Learning at a Distance: Experiences with Tango,”** Presentation at *Teaching Tools’97*, Syracuse University, Syracuse, NY, November 1997.

   Abstract: Currently we are teaching a section of the computational science course “Programming for the Web” to a group of students at Jackson State University at Jackson, Mississippi. What makes this course unique is that twice a week we “meet” with our students online and present lecture slides, show programming examples, and discuss concepts (in real time) over the Internet. This is made possible by a software system called Tango, a collaborative teaching tool developed at the Northeast Parallel Architectures Center at Syracuse University. This talk will describe our experiences teaching this course, what worked, and what didn’t. More generally, we will speculate on the future of distance–learning technologies and barriers to change in the educational marketplace.

3. D. Dias, G.C. Fox, W. Furmanski, V. Mehra, B. Natarajan, H.T. Ozdemir, S. Pallickara, Z. Ozdemir, **“Exploring JSDA, CORBA and HLA based MuTech’s for Scalable Televirtual (TVR) Environments,”** Presented at the Workshop on OO and VRML, *VRML98 Conference*, Monterey, CA, February 1998, http://www.cs.uni–sb.de/~diehl/workshop/proc.html.

   Abstract: We discuss here new distributed computing technologies of relevance for building multi–user scalable televirtual (TVR) environments on the Internet such as: Java Shared Data API (JSDA) by JavaSoft, Common Object Request Broker Architecture (CORBA) by Object Management Group (OMG) and High Level Architecture (HLA) by Defence Modeling and Simulation Office (DMSO). We describe our early TVR prototype based on VRML2 front–end and JSDA back–end, and we summarize our ongoing work on exploring CORBA Events and HLA Dynamic Data Distribution technologies for building scalable collaboration servers for the Internet.

4. Panel Discussion: T.R. Scavo, **“Collaborative and Web–Based Tools,”** High Performance Computing Applications and Technology Symposium, Clark–Atlanta University, Atlanta, GA, March 1998.

5. G.C. Fox, W. Furmanski and H.T. Ozdemir, **“JWORB – Java Web Object Request Broker for Commodity Software based Visual Dataflow Metacomputing Programming Environment,”** Submitted for the *HPDC–7*, Chicago, IL, July 1998, http://tapetus.npac.syr.edu/iwt98/pm/documents/hpdc98/paper.html.

   Abstract: JWORB is a multi–protocol Java server under development at NPAC, currently capable of handling HTTP and IIOP prototocols. Hence, JWORB can be viewed as a Java based Web Server which can also act as a CORBA broker. We present here JWORB rationale, architecture, implementation status, results of early performance measurements and we illustrate its role in the new WebFlow system under development.

6. G.C. Fox, W. Furmanski, B. Natarajan, H.T. Ozdemir, Z. Odcikin Ozdemir, S. Pallickara and T. Pulikal, **“Integrating Web, Desktop, Enterprise and Military Simulation Technologies To Enable World–Wide Scalable Televirtual (TVR) Environments,”** Submitted to the Workshop on Web–based Infrastructures for Collaborative Enterprises, the *WET ICE’98 Conference*, Stanford University, Stanford, CA, June 1998, http://osprey7.npac.syr.edu:1998/iwt98/projects/webhla/users/hasan/papers/WETICE/paperWETICE.html.

   Abstract: We present an approach to the next generation televirtual (TVR) environments that integrate collaboration with distributed computing and modern modeling and simulation technologies. We follow the 3–tier architecture with the Web Object (Java/CORBA) based middleware, VRML/Java3D/DirectX based front–ends and JDBC/PSS/OLEDB based back–ends and we are testing our design and the integration concepts by prototyping a multi–user authoring and runtime environment to support WebHLA based distributed military simulations. We present first our taxonomy of collaboratory frameworks and our integration paradigm, based on the WebFlow system at NPAC. We then list the critical enabling technologies that are being integrated and finally we summarize the current status of our prototyping experiments.

7. D. Bernholdt, G.C. Fox, W. Furmanski, B. Natarajan, H.T. Ozdemir, Z. Odcikin Ozdemir and T. Pulikal, **“WebHLA – An Interactive Programming and Training Environment for High Performance Modeling and Simulation,”** Submitted to the *DoD HPC Users Group Conference*, Houston, TX, June 1998, http://tapetus.npac.syr.edu/iwt98/pm/conferences/DoDHPC98UGC/Abstract.htm.

   Abstract: Our technology roadmap for High Performance Modeling and Simulation, outlined in NPAC PET FMS White Paper is based on three ongoing and rapid technology evolution processes:

- transition of the DoD M&S standards from DIS to HLA
- extension of Web technologies from passive information dissemination to interactive distributed computing based on enterprise standards offered by CORBA, Java and DCOM
- transition of HPCC systems from custom (such as dedicated MPPs) to commodity base (such as NT clusters)

One common aspect of all these threads is the enforcement of reusability and shareability of products or components based on new technology standards. DMSO HLA makes the first major step in this direction by offering the interoperability framework between a broad spectrum of simulation paradigms, including both real–time and logical time models. However, HLA leaves several implementation decisions open and to be made by the application developers – this enables reusability and integrability of existing codes but often leaves developers of new simulations without enough guidance. In WebHLA, we fill this gap by using the emergent standards of Web based distributed computing, referred by some as the Object Web that integrate Java, CORBA, W3C and DCOM models for distributed componentware. Traditional HPCC, dominated by data parallel MPP didn't make significant inroads into the DoD M&S where the focus is on task parallel heterogeneous distributed computing. Recent trends towards commodity based HPCC systems such as NT clusters offer a new promising framework for new generation high performance high fidelity M&S environments such as addressed by JSIMS, JWARS, JMASS or Wargame2000 programs. We therefore believe that WebHLA, defined as the convergence point of the standardization processes outlined above will offer a powerful modeling and simulation framework, capable to address the new challenges of DoD computing in the areas of Simulation Based Design, Testing, Evaluation and Acquisition.

8. E. Akarsu, G.C.Fox, W. Furmanski, T. Haupt, H. Ozdemir, Z. Odcikin Ozdemir, S. Pallickara and T. Pulikal, **"Building Web/Commodity based Visual Authoring Environments for Distributed Object/Component Applications – A Case Study using NPAC WebFlow System,"** Submitted to *Middleware '98, IFIP International Conference on Distributed Systems Platforms and Open Distributed Processing*, The Lake District, United Kingdom, September 1998, http://www.npac.syr.edu/projects/webspace/doc/middleware98/

   Abstract: We present here an approach towards visual authoring environments for Web/Commodity based distributed object/componentware computing using the WebFlow system under development at NPAC as a case study. WebFlow is a 3–tier Java based visual dataflow system with applets based authoring, visualization and control front–ends, and with servlets based middleware management of backend modules that wrap legacy codes such as databases or high performance simulations. We summarize here the WebFlow architecture, we describe a set of demos and early applications in various areas of distributed computing (including imaging, collaboration, condensed matter physics and military wargaming simulations), and we outline the next phase design, based on lessons learned in the current prototype. New WebFlow uses JWORB (Java Web Object Request Broker) middleware and employs WOMA (Web Object Management Architecture) methodology to establish a testbed for testing, evaluating and integrating the emergent componentware standards of CORBA, DCOM, Java and W3C/WOM.

9. G. Fox and W. Furmanski, **"HPcc as High Performance Commodity Computing,"** Book Chapter in *Building A National Grid*, edited by I. Foster and C. Kesselman, Morgan and Kaufman, 1998, http://www.npac.syr.edu/users/gcf/HPcc/HPcc.html.

   Abstract: We review the growing power and capability of commodity computing and communication technologies largely driven by commercial distributed information systems. These systems are built from CORBA, Microsoft's COM, Javabeans, and less sophisticated web and networked approaches. One can abstract these to a three–tier model with largely independent clients connected to a distributed network of servers. The latter hosts various services including object and relational databases and of course parallel and sequential computing. High performance can be obtained by combining concurrency at the middle server tier with optimized parallel backend services. The resultant system combines the needed performance for large–scale HPcc applications with the rich functionality of commodity systems. Further the architecture, with distinct interface, server and specialized service implementation layers, naturally allows advances in each area to be easily incorporated. We show that this approach can be applied to both metacomputing and to provide improved parallel programming environments. We describe exploitation issues within a CORBA context and illustrate how performance can be obtained within a commodity architecture. Examples are given from collaborative systems, support of multidisciplinary interactions, proposed visual HPcc ComponentWare, distributed simulation and the use of Java in high performance computing.

10. G. C. Fox, W. Furmanski and S. Pallickara, **"Building Distributed Systems for the Pragmatic Object Web,"** Wiley, 1998, in progress, http://www.npac.syr.edu/users/shrideep/book/.

    Abstract: This book does not discuss any particular software technology in detail. There are many excellent existing books on Java, CORBA and so on – the widgets from which the Pragmatic Object Web is built. We assume the reader will turn to these for any given particular knowledge area. Rather we assume that the software juggernaut will continue to evolve but somehow converge to what we term the Object Web. This combines the distributed object management model of CORBA, the visual programming of activeX and Javabeans, and the universal deployment of the Web. Today we can only see a fragmented distorted view of this express train to software heaven but suggest that one can identify a "Pragmatic Object Web". This is a mosaic of emerging software technologies which can build distributed systems which are at times flaky and incomplete but offer significant advantages over competing approaches.

    The Object Web is built on universal interfaces allowing not just component re–use but more importantly integration of "systems of (sub)systems" of unprecedented power. The Object Web offers software components that are higher level and hence more powerful that those of previous system building methodologies. For instance JDBC (Java Database Connectivity) allows one to view a database as a system widget — a larger subsystem than that embodied in say X or Motif. Such large grain size components with universal interfaces allow major increases in programmer productivity that can cut software development costs significantly.

    We have designed this book to be read standalone by those interested in distributed systems. It can also be used in training or University curricula where the book provides a framework or architecture for a set of courses covering the individual technologies in great detail.

Tables

Table 1
TECHNICAL SUPPORT TEAM PERSONNEL

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
ERC (Mississippi State) — LEADERSHIP						
Joe Thompson, PhD	MSU	At University	Distinguished Professor	Academic Team Lead	61	77
Alisha Davis	MSU	At University	Technical Information Processor	Administrative Support	30	0
ERC (Mississippi State) — CFD, some SPPT & SV						
David Huddleston, PhD	MSU	At University	Associate Professor	CFD Academic Lead	26	24
Steve Bova, PhD	MSU	On–Site	Research Engineer	CFD On–Site Lead	100	All
Jianping Zhu, PhD	MSU	At University	Professor	CFD code parallelization	31	14
Raghu Machiraju, PhD	MSU	At University	Assistant Professor	SV	10	5
Anthony Skjellum, PhD	MSU	At University	Associate Professor	SPPT–MPI	3	2
Shane Hebert	MSU	At University	Research Assistant	SPPT–MPI	18	8
Brian Jean	MSU	At University	Research Assistant	Grid codes	23	29
Puri Bangalore	MSU	At University	Research Assistant	CFD code parallelization	53	17
Clarence Burg	MSU	At University	Graduate Student	Programmer	0	2

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
NCSA (Illinois) & ERC (Mississippi State) — CSM						
LeRay Dandy	NCSA	At University	DoD Team Leader—Computational Structural Mechanics	CSM Academic Lead	50 as of 11/97	9
Richard Weed, PhD	MSU	On–Site	Research Engineer	CSM On–Site Lead	100	All
Bruce Loftis, PhD	NCSA	At University	Computational Scientist	CSM visualization application development & CSM code optimization	15	1
John Towns	NCSA	At University	Associate Director, Scientific Computing Division	Project development & HDF	5	3
Christina Beldica, PhD	NCSA	At University	Post Doctoral Research Associate	Tracking, web development and develop CSM user applications	20	0
Youngjin Woo	NCSA	At University	Graduate Research Assistant	CSM applications development	50	0
Gyuseok Kwak	NCSA	At University	Graduate Research Assistant	CSM applications development	50	0

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Ohio State — CWO						
P. Sadayappan, PhD	Ohio State	At University	Professor	CWO code parallelization		12
Keith Bedford, PhD	Ohio State	At University	Professor	CWO Academic Lead	10	12
David J.S. Welsh, PhD	Ohio State	At University	Senior Research Associate–Engineer	WAM support and coupling with CH3D, MM5, COSED and FBM	58 as of 9/97	12
Shuxia Zhang	Ohio State	At University	Research Scientist	Support CH3D, SED, MM5 & MPI	67 as of 8/97	2
Sean O’Neil	Ohio State	At University	Research Scientist			0
TICAM (Texas) — EQM						
Mary F. Wheeler, PhD	Texas	At University	Professor	EQM Academic Lead	25	14
Clint Dawson, PhD	Texas	At University	Associate Professor	Co–Lead	25	11
Victor Parr, PhD	Texas	At University	Consultant	Programmer	100	9
Monica Martinez, PhD	Texas	At University	Research Associate	Parallelization of ADCIRC	33	3
Carter Edwards	Texas	At University	Research Associate	Mesh Partitioning Tools	17	3

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Srinivas Chippada	Texas	At University	Research Associate	Parallelization of CE–QUAL–ICM and ADCIRC	42	0
Steve Bryant	Texas	At University	Research Faculty	Development of PARSSIM	16.7	0
Sujatha Sagiraju	Texas	At University	Research Assistant	Launching of PARSSIM	58	0
Robert McLay	Texas	At University	Research Associate	Launching of PARSSIM	33	0
Joe Eaton	Texas	At University	Research Assistant	Mesh Partitioning Algorithm	8	0
Jennifer Proft	Texas	At University	Research Assistant	CE–QUAL–ICM	8	0
Stephanie Tomlinson	Texas	At University	Undergraduate Assistant	Web Pages	25	0
Connie Baxter	Texas	At University	Administrative Associate	Staff Support	25	0
Sarah Woodruff	Texas	At University	Administrative Assistant	Assistant to Connie Baxter	25	0
NPAC (Syracuse) — FMS & C/C						
Geoffrey Fox, PhD	Syracuse	At University	Professor & Director, NPAC	Academic Lead	Total .29 FTE	4
David Bernholdt, PhD	Syracuse	At University	Research Scientist	Project Leader		6
Tom Scavo	Syracuse	At University	Research Scientist	Project Leader, Computational Science Education	Total .63 FTE	0
Nancy McCracken, PhD	Syracuse	At University	Sr. Research Scientist	Computational Science Education		4
Saleh Elmohamed	Syracuse	At University	Graduate Research Assistant	Computational Science Education		0

Team Member	Affiliation	Location	Title	Role	% Time	Days On-Site
Meryem Ispirli	Syracuse	At University	Graduate Research Assistant	Computational Science Education		0
Mehmet Sen	Syracuse	At University	Graduate Research Assistant	Computational Science Education		0
Marek Podgorny, PhD	Syracuse	At University	Associate Director NPAC	Project Leader, Tango Collaboratory Group	Total 3.19 FTE	0
Roman Markowski	Syracuse	At University	Information Systems Manager NPAC	Tango Collaboratory Group		0
Lukasz Beca	Syracuse	At University	Graduate Research Assistant	Tango Collaboratory Group		4
Tomasz Jurga	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0
Grzegorz Lewandowski	Syracuse	At University	Graduate Research Assistant	Tango Collaboratory Group		0
Tomasz Major	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0
Konrad Olszewski	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0
Piotr Sokoloski	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0
Pawel Roman	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0
Tomasz Stachowiak	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0
Remigiusz Trzaska	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Bartlomiej Winnowicz	Syracuse	At University	Research Scientist	Tango Collaboratory Group		0
Wojtek Furmanski, PhD	Syracuse	At University	Reserach Professor	Project Leader, Interactive Web Technologies Group	Total .64 FTE	0
Ozgur Balsoy	Syracuse	At University	Graduate Research Assistant	Interactive Web Technologies Group		0
Tomasz Haupt	Syracuse	At University	Research Scientist	Interactive Web Technologies Group		1
Scott Klasky	Syracuse	At University	Research Scientist	Interactive Web Technologies Group		2
Hasan Ozdemir	Syracuse	At University	Graduate Research Assistant	Interactive Web Technologies Group		0
Zeynep Ozdemir	Syracuse	At University	Graduate Research Assistant	Interactive Web Technologies Group		0
Chao–Wei Ou	Syracuse	At University	Research Scientist	Database Applications Group	Total .57 FTE	0
Yuping Zhu	Syracuse	At University	Research Scientist	Database Applications Group		2
Todd Olson	Syracuse	At University	Data Systems Administrator	Technical and Administrative Support	Total .27 FTE	0
Dona Sobotka	Syracuse	At University	Administrative Specialist III	Technical and Administrative Support		0

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
NCSA (Illinois) — C/C						
Lex Lane	NCSA	At University	Associate Director	C/C Academic Lead	10 (11/97 – 3/98)	5
Sandie Kappes	NCSA	At University	Research Programmer	C/C Team Leader	33 (11/97 – 3/98)	5
Lisa Gatzke	NCSA	At University	Hypermedia Communicator	Web Designer	33 (4/97 – 3/98	0
Frank Baker	NCSA	At University	Hypermedia Communicator	C/C Academic Lead	33 (4/97 – 12/97)	2
John Ziebarth, PhD	NCSA	At University	Associate Director for Education & Outreach	C/C Senior Academic Lead	7 (4/97 – 6/97)	2
Alan Craig	NCSA	At University	Research Programmer	netWorkPlace Project Leader	10 (4/97 – 6/97)	0
Tom Prudhomme, PhD	NCSA	At University	Associate Director of Government Programs	Management	11 (11/97 – 3/98)	1
Mary Bea Walker	NCSA	At Univesity	DoD MSRC PET Program Manager	Management	10 (4/97 – 3/98)	0
Annette Felkner	NCSA	At University	Budget Analyst	Budget Analyst	10 (4/97 – 3/98)	0
CRPC (Rice, Tennessee) — SPPT						
Ken Kennedy, PhD	Rice	At University	Professor	Senior Academic Lead SPPT	4.5	0
Charles Koelbel, PhD	Rice	At University	Research Scientist II	Academic Lead SPPT	23.6	9

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Clay P. Breshears, PhD	Rice	On–Site	Research Scientist	On–Site Lead SPPT	100 since 6/16/97	All
Logan Ratner	Rice	At University	Systems Programmer	Web Maintainer	5	0
Gina Goff, PhD	Rice	At University	Research Programmer	Technology Tracker	50	3
Ehtesham Hayder, PhD	Rice	At University	Research Scientist II	Technology Tracker	33 since 10/1/97	5
Shirley Browne, PhD	Tennessee	At University	Associate Director of Research	Lead for Debugging and Performance Tools Focused Effort, Coordination of UTK Participation in CEWES MSRC PET	60	16
Susan Blackford	Tennessee	At University	Research Associate	Installation, Testing, Timing, and Training on Numerical Libraries	20	4
Clint Whaley	Tennessee	At University	Research Associate	Testing and Bug Reporting onSystems and Library Software, Port of ScaLAPACK to Cray T3E	10	0
Victor Eijkhout, PhD	Tennessee	At University	Research Assistant Professor	Evaluation of and Training on Sparse Linear Algebra Solver Packages	6	4
Erich Strohmaier, PhD	Tennessee	At University	Research Associate	Performance Evaluation	50	3
Phil Mucci	Tennessee	At University	Research Associate	Performance Evaluation	50	7

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Andrew Rogers	Tennessee	At University	Undergraduate Student Assistant	Performance Evaluation	25	0
Kevin London	Tennessee	At University	Computer Specialist	Debugging and Performance Tools, MPI Interconnection and Control, Performance Evaluation	50	12
John Thurman	Tennessee	At University	Graduate Research Assistant	Performance Evaluation	12.5	0
Graham Fagg, PhD	Tennessee	At University	Senior Research Associate	MPI Interconnection and Control	2.8	7
Micah Beck, PhD	Tennessee	At University	Research Assistant Professor	MPI Interconnection and Control	6	0
Martin Swany	Tennessee	At University	Research Associate	Debugging and Performance Tools, MPI Interconnection and Control	12.5	0
Paul McMahan	Tennessee	At University	Program Director	Interoperable CTA Software Repositories	8.3	0
Scott Wells	Tennessee	At University	Research Associate	Interoperable CTA Software Repositories	5	0
Arun Rattan	Tennessee	At University	Graduate Research Assistant	Performance Evaluation	12.5	0
Rana Darmara	Rice	At University	Contract Administrator	Administration and Clerical Support	10	0
Danny Powell	Rice	At University	Business Manager	Administration and Clerical Support	10	0
Kathryn O’Brien	Rice	At University	Administrative Assistant	Administration and Clerical Support	15	0

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Joe Sowa	Rice	At University	Bookkeeper	Administration and Clerical Support	5	0
Doug Hewett	Rice	At University	Bookkeeper Assistant	Administration and Clerical Support	5	0
Corina Cardenas	Rice	At University	Administrative Assistant	Administration and Clerical Support	4.6	0
Tracy Rafferty	Tennessee	At Univeristy	Grants and Contracts Specialist	Administration and Clerical Support	10	0
NCSA (Illinois) & NRC — SV						
Polly Baker, PhD	NCSA	At University	Senior Research Scientist	Senior SV Academic Lead	20	16
Richard Strelitz, PhD	SAIC	On–Site	S**K Head	SV On–Site Lead (since 1/98)	100	All
Alan Shih, PhD	NCSA	At University	Research Scientist	SV Site Lead (since 1/98)	100	18
Jay Jackson, PhD	NCSA	At University	Research Scientist	SV Site Lead (summer 97)	75	5
Rob Stein	NCSA	At University	Visualization Programmer	Project Developer	50	3
Randy Heiland	NCSA	At University	Visualization Programmer	Project Devloper	65	3
Dave Bock	NCSA	At University	Visualization Programmer	Project Developer	40	0
Alan Craig	NCSA	At University	Visualization Programmer	Project Developer	30	0
Ed Peters	NCSA	At University	Graduate Student	Project Developer	50	3

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Tom Prudhomme, PhD	NCSA	At University	Associate Director	University Liaison	8	6
Jackson State University						
Willie G. Brown, PhD	JSU	At University	Chairman, Department of Computer Science, Assistant Vice President for Information Technology	Director of PET activities for JSU (HBCU Lead University)	25	9
Carolyn Laury	JSU	At University	Administrative Assistant	Provides clerical support for JSU PET activities	100	0
Mildred Leonard	JSU	At University	Scientific Visualization Specialist	Works on remote scientific visualization projects in collaboration with NCSA and the CEWES MSRC. Also provides training to JSU students and faculty, and DoD users.	100	9
Edgar Powell	JSU	At University	Scientific Visualization Technologist	Provides technical support for the scientific visualization effort at JSU and the CEWES MSRC	100	4
Michael Robinson	JSU	At University	Network Training Specialist	Provides technical support for Web–Based Distance education effort at JSU in collaboration with NPAC	100	0

Team Member	Affiliation	Location	Title	Role	% Time	Days On–Site
Clark Atlanta University						
O. Olatidoye, PhD	CAU	At University	Associate Professor	PI, Residual capacity evaluation & visualization		
S. Sarathy, PhD	CAU	At University	Assistant Professor	Co–PI	20	15
G. Jones	CAU	At University	Student	Co–PI	33	2

Table 2 TEAM TRAVEL				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
ERC (Mississippi State) — LEADERSHIP				
CEWES MSRC	MSU	Thompson	77	On–Site at CEWES MSRC
Rice University	MSU	Thompson	2	PET Executive Committee Meeting
San Jose, CA	MSU	Thompson	7	Supercomputing ’97
Portand, OR	MSU	Thompson	4	Timberline PET Planning Meeting
San Diego, CA	MSU	Thompson	5	DoD HPCMP User Group Meeting
Washington, DC	MSU	Thompson	2	Meet with Dr. Anita Jones on DoD PET Program
University of Texas	MSU	Thompson	4	CEWES MSRC Joint CTA Workshop on Grid Generation Issues
ERC (Mississippi State) — CFD (some SV & SPPT)				
CEWES MSRC	MSU	Huddleston	2	Mississippi Section ASCE Spring ’97 Meeting
CEWES MSRC	MSU	Huddleston	3	CEWES MSRC PET Annual Review
ASC MSRC	MSU	Huddleston	4	MAPINT ’97
San Diego, CA	MSU	Huddleston	5	DoD HPCMP User Group Meeting
Snowmass, CO	MSU	Huddleston	4	AIAA CFD Conference (Shared funding)
San Francisco, CA	MSU	Huddleston	5	ASCE Water Resources Conference (Shared funding)
CEWES MSRC	MSU	Huddleston	2	CEWES MSRC PET Mid–Year Review
CEWES MSRC	MSU	Huddleston	2	CEWES MSRC PET Annual Review
CEWES MSRC	MSU	Huddleston	5	CEWES MSRC PET Contract Support

Destination	Institution	PET Personnel	Duration (Days)	Purpose
San Diego, CA	MSU	Zhu	5	DoD HPCMP User Group Meeting
CEWES MSRC	MSU	Zhu	2	CEWES MSRC PET Mid–Year Review
CEWES MSRC	MSU	Zhu	1	CEWES MSRC PET Annual Review
San Jose, CA	MSU	Zhu	6	Supercomputing ’97
CEWES MSRC	MSU	Zhu	5	On–Site at CEWES MSRC
Mississippi State University	MSU	Bova	2	Third MSU Conference on Differential Equations and Computational Simulations
Plymouth, NH	MSU	Bova	5	Gordon Research Conference on High Performance Computing and Information Infrastructure
San Diego, CA	MSU	Bova	5	DoD HPCMP User Group Meeting
Snowmass, CO	MSU	Bova	4	AIAA CFD Conference (Shared Funding)
Mississippi State University	MSU	Bova	2	ERC Industrial Affiliates Meeting
San Jose, CA	MSU	Bova	6	Supercomputing ’97
CEWES MSRC	MSU	Bangalore	1	CEWES MSRC PET Contract Support
Boston, MA	MSU	Machiraju	6	Industrial Contacts for Terascale Visualization Project
CEWES MSRC	MSU	Bangalore	1	CEWES MSRC PET Year 3 Proposal Meeting
CEWES MSRC	MSU	Bangalore	4	CEWES MSRC PET Annual Review
CEWES MSRC	MSU	Bangalore	4	Course on Code Optimization for MPPS
San Jose, CA	MSU	Bangalore	9	Supercomputing ’97
CEWES MSRC	MSU	Bangalore	5	CFD Group Meeting and Present MPI Tutorial
CEWES MSRC	MSU	Bangalore	2	CEWES MSRC PET Mid–Year Review
NRL	MSU	Bangalore	5	Present MPI Tutorial at NRL

Destination	Institution	PET Personnel	Duration (Days)	Purpose
NRL	MSU	Bangalore	5	Present the Message Passing Interface Tutorial at NRL
University of Texas	MSU	Bova	5	CEWES MSRC Joint CTA Workshop on Grid Generation Issues
Reno, NV	MSU	Bova	4	36th Annual AIAA Aerospace Sciences Meeting
San Jose, CA	MSU	Bova	7	Supercomputing ’97
NRL	MSU	Bova	5	Conduct Workshop on HPC at NRL
Mississippi State University	MSU	Bova	3	IA Meeting at MSU
Mississippi State University	MSU	Bova	2	Meet with ERC Personnel Prior to Semi–Annual CEWES MSRC PET Review
Albuquerque, NM	MSU	Bova	3	Meet with CEWES MSRC Users
Plymouth, NH	MSU	Bova	5	Gordon Research Conference on HPC
San Diego, CA, Snowmass, CO	MSU	Bova	10	San Diego: DoD HPCMP User Group Meeting, Snowmass: AIAA CFD Meeting
Mississippi State University	MSU	Bova	3	MSU Conference on Differential Equations and Computational Simulations
CEWES MSRC	MSU	Burg	2	Presentation at CEWES MSRC
CEWES MSRC	MSU	Hebert	1	CEWES MSRC PET Year 3 Proposal Meeting
CEWES MSRC	MSU	Hebert	5	Present MPI Tutorial
NRL	MSU	Hebert	5	Teach MPI Tutorial at NRL
NRL	MSU	Hebert	5	Teach MPI Tutorial at NRL
NRL	MSU	Hebert	5	Teach MPI Tutorial at NRL
CEWES MSRC	MSU	Huddleston	3	CEWES MSRC PET Annual Review
CEWES MSRC	MSU	Huddleston	2	CEWES MSRC PET Contract Support

Destination	Institution	PET Personnel	Duration (Days)	Purpose
CEWES MSRC	MSU	Huddleston	2	CEWES MSRC PET Contract Support
CEWES MSRC	MSU	Huddleston	1	CEWES MSRC PET Contract Support
San Francisco, CA	MSU	Huddleston	5	27th International Assoc. of Hydraulic Research Congress
CEWES MSRC	MSU	Huddleston	1	CEWES MSRC PET Contract Support
San Diego, CA, Snowmass, CO	MSU	Huddleston	10	San Diego, Present at DoD HPCMP User Group Meeting, Snowmass: AIAA CFD Conference
ASC MSRC	MSU	Huddleston	4	CEWES MSRC PET Contract Support
CEWES MSRC	MSU	Huddleston	1	CEWES MSRC PET Contract Support
CEWES MSRC	MSU	Jean	27	Grid Code Evaluation for CEWES MSRC PET
Park City, UT	MSU	Jean	3	Attend 6th Int'l Meshing Roundtable
CEWES MSRC	MSU	Jean	2	Grid Software Installation at CEWES MSRC
CEWES MSRC	MSU	Machiraju	1	CEWES MSRC PET Contract Work
University of Texas	MSU	Machiraju	3	CEWES MSRC Joint CTA Workshop on Grid Generation Issues
CEWES MSRC	MSU	Machiraju	2	Meet with Engineers at CEWES MSRC
CEWES MSRC	MSU	Machiraju	2	Attend Roundtable Conference on Scientific Visualization
CEWES MSRC	MSU	Skjellum	1	Attend CEWES MSRC PET Year 3 Proposal Meeting
NRL	MSU	Skjellum	5	Conduct Training for MPI at NRL
CEWES MSRC	MSU	Skjellum	1	CEWES MSRC PET Contract Work
CEWES MSRC	MSU	Zhu	1	CEWES MSRC PET Annual Review
San Jose, CA	MSU	Zhu	4	Present Poster Exhibit at Supercomputing '97
CEWES MSRC	MSU	Zhu	1	Meeting of CFD, Environment Quality Modeling and Computational Weather Forecasting Groups

Destination	Institution	PET Personnel	Duration (Days)	Purpose
CEWES MSRC	MSU	Zhu	2	Meeting of CEWES MSRC PET Groups
CEWES MSRC	MSU	Zhu	2	CEWES MSRC PET Annual Review
San Diego, CA	MSU	Zhu	4	DoD HPCMP User Group Meeting
CEWES MSRC	MSU	Bova	2	Work with MSU Personnel on CEWES MSRC PET Contract
CEWES MSRC	MSU	Huddleston	2	CEWES MSRC PET Contract Support
NCSA (Illinois) and ERC (Mississippi State) — CSM				
AEDC	MSU	Weed	5	Conduct Parallel Programming Workshop at Arnold Air Force Base, TN
San Jose, CA	MSU	Weed	5	Supercomputing ’97
Mississippi State University	MSU	Weed	3	IA Meeting
Williamsburg, VA	MSU	Weed	5	4th Natn’l Symposium on Large Scale Analysis and Design on HPC and Workstations
Minneapolis, MN	MSU	Weed	3	Unstructured Mech. Generation and Partitioning Workshop
NCSA	MSU	Weed	2	Meet with NCSA to discuss CEWES MSRC PET
Albuquerque, NM	MSU	Weed	4	Briefings for Phillips Labs and Kirkland AFB on CEWES MSRC PET
San Diego, CA	MSU	Weed	5	DoD HPCMP User Group Meeting
ARL MSRC	MSU	Weed	2	CHSSI Meeting
AEDC	MSU	Weed	4	Workshop on Designing & Building Parallel Programs
Mississippi State University	MSU	Weed	1	New Employee Orientation
CEWES MSRC	NCSA	Dandy, Loftis	1	Meet CSM users at CEWES MSRC: Raju Namburu, Steve Akers, and Robert Hall

Destination	Institution	PET Personnel	Duration (Days)	Purpose
CEWES MSRC	NCSA	Dandy	3	CTH training class and meet with CTH users (Raju Namburu, Jon Windham, Doug Strasburg) to discuss developing new material model, meet CSM users at CEWES MSRC
CEWES MSRC	NCSA	Dandy	2	Meet CSM users at CEWES, attend grid workshop at UT Austin
CEWES MSRC	NCSA	Dandy, Towns	3	Meet CSM users at CEWES MSRC, CEWES MSRC PET Annual Review
Ohio State — CWO				
CEWES MSRC	Ohio State	Welsh, Bedford, Sadayappan, Zhang	4	OSU personnel learned basics about running WAM at CEWES MSRC, discussion concerning restart requirements for parallel WAM, discussion of strategy for coupling of WAM and CH3D.
Alexandria, VA	Ohio State	Bedford, Zhang, O'Neil	3	Attended 5th International Conference on Estuarine and Coastal Modeling and met with experts in the field of Lake Michigan hydrodynamic modeling (e.g., Drs. David Schwab and Dmitry Belestkey of NOAA GLERL) to discuss the rquirements and benefits of applying the CH3D–SED model to that lake.
University of Texas	Ohio State	Bedford, Zhang, O'Neil	3	Attended PET grid–workshop at Univ. of Texas–Austin and discussed the gridding problem that was faced in developing a fully coupled current circulation, wave and sediment transport simulation system.
CEWES MSRC	Ohio State	Welsh, Bedford, Sadayappan	4	Attended CEWES MSRC PET year end meeting, made presentation on progress of WAM/CH3D coupling, discussed WAM/CH3D with Bob Jensen, planned deployment of WAM on each CEWES MSRC platform and associated testing, discussed with Graham Fagg of U. of Tennessee the use of PVMPI for WAM/CH3D synchronization in a cross–platform environment

Destination	Institution	PET Personnel	Duration (Days)	Purpose
CEWES MSRC	Ohio State	Bedford, Sadayappan, Welsh	4	CEWES MSRC PET Annual Review and Planning Meeting
TICAM (Texas) — EQM				
CEWES MSRC	Texas	Wheeler	3	CEWES MSRC PET Annual Review
CEWES MSRC	Texas	Parr	4	Delivered CE–QUAL–ICM Version 1.0 and Trained CEWES personnel
CEWES MSRC	Texas	Wheeler, Dawson, Parr	2	Delivered CE–QUAL–ICM Version 1.1, Interviewed Robert Fithen for On–Site Lead
CEWES MSRC	Texas	Wheeler, Dawson	2	Meeting with CEWES EQM personnel on Future Goals: Holland, Dortch, Cerco, etc.
CEWES MSRC	Texas	Wheeler, Dawson, Parr, Martinez, Edwards	3	Workshop on Parallel Technology
Rice Univesity	Texas	Wheeler	3	PET Executive Committee Meeting
CEWES MSRC	Texas	Wheeler, Dawson	4	CEWES MSRC PET Annual Review
NPAC (Syracuse) — FMS & C/C				
CEWES MSRC	Syracuse	Bernholdt	1	CEWES MSRC PET Annual Review
San Diego, CA	Syracuse	Bernholdt, Fox, Furmanski	5	DoD HPCMP User Group Meeting
CEWES MSRC	Syracuse	Beca, McCracken	4	Java Training (Distance Education Pilot)
CEWES MSRC	Syracuse	Fox	1	Seminar and Discussions
Jackson State University	Syracuse	McCracken, Podgorny, Scavo, Stachowiak	3	Distance Education Course Kick–Off
Jackson State University	Syracuse	Scavo	2	Distance Education Course Check–Up
CEWES MSRC	Syracuse	Bernholdt, Zhu	2	Discussions of Web–Linked Database Projects
Jackson State University	Syracuse	McCracken	1	Distance Education Course Check–Up

Destination	Institution	PET Personnel	Duration (Days)	Purpose
Jackson State University	Syracuse	Scavo	3	Distance Education Course Final Projects
Jackson State University	Syracuse	Scavo	2	Distance Education Course Kick–Off
CEWES MSRC	Syracuse	Klasky	2	Scientific Visualization Meeting
CEWES MSRC	Syracuse	Haupt	1	Meeting with Jeff Holland
Rice University	Syracuse	Fox	3	Cross–MSRC Training Group & PET Executive Committee
University of Texas	Syracuse	Zhu	2	CEWES MSRC Joint CTA Workshop on Grid Generation Issues
CEWES MSRC	Syracuse	Bernholdt, Fox	3	CEWES MSRC PET Annual Review
Jackson State University	Syracuse	Scavo	2	Distance Education Course Check–Up
NCSA (Illinois) — C/C				
CEWES MSRC	NCSA	Ziebarth, Baker, Ferguson	2	CEWES MSRC PET Annual Review
Syracuse University	NCSA	Baker	2	TANGO Training
San Diego, CA	NCSA	Craig, Baker, Ziebarth, Ferguson, Walker	5	DoD HPCMP User Group Meeting. Craig presented workshop on collaborative software environments. Others attended in support of various PET activities.
CEWES MSRC	NCSA	Kappes, Lane	2	Site Visit to Discuss C/C User Requirements
CEWES MSRC	NCSA	Kappes, Lane	3	CEWES MSRC PET Annual Review
CRPC (Rice, Tennessee) — SP				
CEWES MSRC	Tennessee	Browne	4	CEWES MSRC PET Annual Review
CEWES MSRC	Rice	Koelbel	4	CEWES MSRC PET Annual Review
Rice University	Rice	Breshears	5	PET Meeting with CRPC Personnel and CRPC Annual Meeting

Destination	Institution	PET Personnel	Duration (Days)	Purpose
Boulder, CO	Tennessee	Browne	8	Parallel Tools Consortium Meeting and Chair Working Group at High Performance Debugging Forum Meeting, Travel Supported 1/3 by CEWES MSRC
CEWES MSRC	Tennessee	Blackford	4	Teach Training Course on Parallel Numerical Libraries
CEWES MSRC	UCLA	Eijkhout	4	Teach Training Course on Parallel Numerical Libraries
Boulder, CO	Tennessee	Browne	4	Chair Working Group at High Performance Debugging Forum Meeting, Travel supported 1/3 by CEWES MSRC
CEWES MSRC	Tennessee	Browne, London	4	CEWES MSRC PET Midyear Review and Work with Breshears on Tools Evaluation
Nashua, NH	Tennessee	Browne	5	Chair Working Group at High Performance Debugging Forum Meeting, Travel supported 1/3 by CEWES MSRC
San Diego, CA	Rice	Breshears, Koelbel	5	DoD HPCMP Users Group Meeting
San Diego, CA	Tennessee	Browne	7	DoD HPCMP Users Group Meeting
CEWES MSRC	Tennessee	Mucci, Strohmaier	3	Teach Training Course on Benchmarking and Performance Evaluation and Meet with CEWES MSRC Personnel about Benchmarking
University of Southern Mississippi	Rice	Breshears	1	Talk by Oscar Naim of University of Wisconsin and ParaDyn Research Group
CEWES MSRC	Tennessee	Fagg	3	Give Seminar at JSU and CEWES MSRC on PVMPI, attend MPI Meeting Organized by Bova
San Jose, CA	Rice	Breshears, Goff, Hayder, Koelbel	6	Supercomputing ’97
San Jose, CA	Tennessee	Browne	7	Present Poster at Supercomputing ’97, Travel supported 60% by CEWES MSRC
San Jose, CA	Tennessee	London	7	Present Poster at Supercomputing ’97

Destination	Institution	PET Personnel	Duration (Days)	Purpose
San Jose, CA	Tennessee	Mucci	7	Present Poster at Supercomputing ’97, Travel supported 50% by CEWES MSRC
San Jose, CA	Tennessee	Horner	7	Present Demo at HPCMO Booth, Travel supported 1/3 by CEWES MSRC
Dallas, TX	Tennessee	Browne	3	Chair Working Group at High Performance Debugging Forum Meeting, Travel supported 1/3 by CEWES MSRC
University of Tennessee	Rice	Breshears	4	BLAS Technical Forum
CEWES MSRC	Rice	Koelbel, Hayder, Goff	2	Meet with CTA Leads and Users to Discuss Code Migration Issues
CEWES MSRC	Tennessee	Browne	4	Teach Workshop on Portable Parallel Performance Tools
CEWES MSRC	Tennessee	London, Mucci	4	Teach Training Course on Code Optimization for MPPs
CEWES MSRC	Rice	Goff	1	SGI/Cray Talks by Peter Rigsbee
CEWES MSRC	Rice	Koelbel, Hayder	3	CEWES MSRC PET Annual Review
CEWES MSRC	Tennessee	Browne, Fagg, London	4	CEWES MSRC PET Annual Review
Mississippi State University	Rice	Breshears, Hayder, Koelbel	1	Meet Researchers at MSU ERC and Tour Facilities
NRL	Rice	Breshears	5	Conduct Parallel Programming (BYOC) Workshop
NCSA (Illinois) — SV				
CEWES MSRC	NCSA	Baker	3	CEWES MSRC PET Annual Review
CEWES MSRC	NCSA	Baker, Stein, Peters	3	User Outreach Meeting
CEWES MSRC	NCSA	Baker, Heiland, Jackson	3	User Outreach Meeting
CEWES MSRC	NCSA	Jackson	2	Conduct Training Class
CEWES MSRC	NCSA	Baker, Shih	3	CEWES MSRC InternalVisualization Workshop

Destination	Institution	PET Personnel	Duration (Days)	Purpose
CEWES MSRC	NCSA	Baker, Shih	4	CEWES MSRC PET Annual Review
San Diego, CA	NCSA	Baker	5	DoD HPCMP User Group Meeting
Portland, OR	NCSA	Baker	3	Timberline PET Planning Meeting
ARL MSRC	NCSA	Baker, Shih, Bock, Strelitz	3	Program–Wide DoD Visualization Workshop
Albuquerque, NM	NCSA	Baker	5	IEEE VR Symposium
Los Angeles, CA	NCSA	Baker, Stein, Peters	7	SIGGRAPH97
Phoenix, AZ	NCSA	Baker	5	IEEE Visualization Conference
San Jose, CA	NCSA	Baker, Heiland, Bock	7	Supercomputing ’97
CEWES MSRC	NCSA	Shih	12	SV Support
Jackson State University				
CEWES MSRC	JSU	Brown, Leonard, Bhalla, Jung, Malluhi, Washington	4	Tango Workshop
CEWES MSRC	JSU	Powell	1	Scientific Visualization Training Session
CEWES MSRC	JSU	Leonard	3	Scientific Visualization Training Session
Portland, OR	JSU	Brown	3	PET Executive Committee, CTA Leaders Workshop

Destination	Institution	PET Personnel	Duration (Days)	Purpose
CEWES MSRC	JSU	Brown	2	CEWES MSRC Mid–Year Review
NCSA	JSU	Leonard	5	Collaboration and Training
San Jose, CA	JSU	Brown	3	Supercomputing ’97
Syracuse, NY	JSU	Robinson	4	Tango Training
Rice	JSU	Brown	3	PET Executive Committee Meeting
CEWES MSRC	JSU	Brown, Leonard, Powell	3	CEWES MSRC Annual Review
Atlanta, GA	JSU	Powell	4	Scientific Visualization Training
NCSA	JSU	Leonard	90	Collaboration
Clark Atlanta University				
CEWES MSRC	CAU		16	Research Status Discussions

Table 3
CEWES MSRC USER CONTACTS

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Bob Jensen	CEWES	CWO	OSU; Bedford, Sadayappan, Welsh	visit to CEWES	Discussion of WAM seamless restart requirements and WAM/CH3D/ COSED coupling strategies.
Billy Johnson	CEWES	CWO	OSU; Zhang	e–mails	Requested and received the CH3D–s code.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mails	Discussion of coding strategies for addition of unsteady current and depth effects in WAM.
Bob Jensen	CEWES	CWO	OSU; Welsh	phone call	Jensen supplied basic CEWES version of WAM.
Billy Johnson	CEWES	CWO	OSU; Zhang	e–mails	Requested and received the WESCORA code, to use for generation of the grid mesh for the CH3D simulation of Lake Michigan.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mail	Copies of OSU CWO mid–year review viewgraphs supplied, plus clarifications of the proposed OSU work plan.
Billy Johnson	CEWES	CWO	OSU; Zhang	e–mail	Zhang reported how the Lake Michigan grid mesh had been generated without the use of the WESCORA code.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Billy Johnson	CEWES	CWO	OSU; Zhang	fax	Sent a map of the Lake Michigan grid mesh in curvilinear coordinates.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mails	Discussed possible reasons for blow–up in WAM STRESSO routine. Problem solved by reducing time step below value previously calculated from Courant condition.
Nolan Rephelt	CEWES	CWO	OSU; Zhang	e–mail and phone calls	Requested and received the CH3D–SED sediment transport code.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mails	Work update requested by Jensen and subsequently supplied; making detailed plans of each WAM code modification required for addition of unsteady current and depth effects.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mails	Discussed meaning of ‘wave’ and ‘total’ stresses in WAM; reached agreement on how the wave stress should be used to modify the wind input in CH3D.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Bob Jensen, Carol Beaty of Cray/SGI	CEWES	CWO	OSU; Welsh	e–mails	Discussion of reasons for slight differences between sequential and parallel WAM results. Possibly due to small algorithm differences between versions.
Bob Jensen, Christine Cuicchi, Carol Beaty of Cray/SGI	CEWES	CWO	OSU; Bedford, Sadayappan, Welsh	visit to CEWES	Attended and made presentation at CEWES MSRC PET year end review meeting. Also formulated plans for establishing equivalent sequential and parallel WAM deployments on the various CEWES MSRC platforms. Discussed verification test for pre–existing WAM current propagation algorithm.
Steve Jones	CEWES	CWO/SV	OSU; Welsh	e–mails	Asked for and received information about suitable image/animation formats for use with ITL 3–screen visualization resource. Conveyed plan to supply CEWES with CWO visualization examples.
Mike Stephens	CEWES	CWO/SV	OSU; Welsh	e–mails	Asked for and received information concerning Stephens' previous use of ITL 3–screen visualization resource.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mail	Jensen supplied clarifications on his ideas for verification of the WAM current propagation algorithm.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mail	Sent copy of OSU CWO bi–weekly report.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mail	Sent color version of OSU CWO focused effort year end report, as requested by Jensen.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mail	Sent copy of OSU CWO abstract submitted to HPCMP Users' Group Conference 1998.
Bob Jensen, Christine Cuichchi, Carol Beaty of Cray/SGI	CEWES	CWO	OSU; Welsh, Sadayappan	e–mails	Wesh requested and received clarification on the OSC T90 runs he agreed to make in order to quantify typical WAM results differences between platforms; this comparison C90 to T90.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Bob Jensen, Christine Cuicchi, Carol Beaty of Cray/SGI	CEWES	CWO	OSU; Welsh, Sadayappan	e–mails	Welsh reported on the results of the T90 WAM runs. It was agreed that the differences between the C90 and T90 results were acceptably small and differences on CEWES MSRC O2K, and T3E platforms should be of a similar order.
Bob Jensen	CEWES	CWO	OSU; Welsh	e–mail	Sent copy of OSU CWO bi–weekly report.
Carl Cerco	CEWES	EQM	Texas	phone, e–mail, and visits	Parallelization of CE–QUAL–ICM.
Mark Noel	CEWES	EQM	Texas	phone, e–mail, and visits	Parallelization of CE–QUAL–ICM.
Barry Bunch	CEWES	EQM	Texas	phone, e–mail, and visits	Parallelization of CE–QUAL–ICM.
Jeff Holland	CEWES	EQM	Texas	phone, e–mail, and visits	EQM projects.
Mark Dortch	CEWES	EQM	Texas	e–mail and visits	Parallelization of CE–QUAL ICM.
Ross Hall	CEWES	EQM	Texas	visits	Parallelization of CE–QUAL ICM–TOXI.
Rao Vemulokanda	CEWES	EQM	Texas	phone, e–mail and visits	parallelization of ADCIRC
Norm Scheffner	CEWES	EQM	Texas	visits	Parallelization of ADCIRC
Fred Tracy	CEWES	EQM	Texas	visit	Discussion of FEMWATER

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Joe Schmidt	CEWES	EQM	Texas	visit	Discussion of groundwater modeling.
Steve Bishop Joe McDonnel Keith Snively	Ft. Belvoir	FMS	Syracuse	visit	Briefing on CMS in conjunction with Year 2 focused effort. This group has since obtained accounts at CEWES MSRC and is porting their code to the Origin2000 there.
Jeff Holland	CEWES	EQM	Syracuse	visit	Discussed prospects for collaboration on 'web launching' of Land Management System modules. Submitted proposal for Year 3 focused effort.
Eileen Viar Geoffrey Sauerborn	ARL	FMS	Syracuse	visit	Discussions of HPC for FMS applications.
David Itkin Henry Ng Roger Nielsen Larry Peterson Mark Roberts Bill Smith Jackie Steele Jeff Steinman Jeff Wallace Bob Wasilausky Alan Whitehurst	SAIC NRL NRL NRaD COLSA NRL SMDC Metron NRaD NRaD (DoD FMS CTA Lead) BYU	FMS	Syracuse	visit	Attended internal review of CHSSI FMS projects.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Carl Cerco	CEWES	EQM	NCSA	visit, phone call, e–mail	Tool development and transfer.
Mark Noel	CEWES	EQM	NCSA	phone call, e–mail	Tool development and transfer.
Bob Jensen	CEWES	CWO	NCSA	visit	User requirements discussion.
Raju Namburu	CEWES	CSM	NCSA	visit	Tool development.
Tommy Bevins	CEWES	CSM	NCSA	visit	Tool development.
Byron Armstrong	CEWES	CSM	NCSA	visit	Tool development.
Photios Papados	CEWES	CSM	NCSA	visit	Tool development.
Mike Stephens	CEWES	SV	NCSA	visit, phone call, e–mail	Joint software development.
Steve Swanekamp	NRL	CFD	CRPC/Rice	personal contact, BYOC workshop	Assisted with code parallization techniques.
Roger M. Oba	NRL	CEA	CRPC/Rice	personal contact, BYOC workshop	Assisted with code parallelization techniques.
Mike Bettenhauser	Mission Research Corp.	CFD	CRPC/Rice	personal contact, BYOC workshop	Assisted with code parallization techniques.
Jerry Sasser	Kirtland AFB	CEA, RF Challenge project	CRPC/Rice, Tennessee	personal contact	Introduced user to available performance analysis tools which were able to be used to identify code inefficiencies.
Sherri Colella	Kirtland AFB	CEA, RF Challenge project	CRPC/Rice, Tennessee	personal contact	Introduced user to available performance analysis tools which were able to be used to identify code inefficiencies.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Larry Merkle	Kirtland AFB	CEA, RF Challenge project	CRPC/Rice, Tennessee	personal contact	Introduced user to available performance analysis tools which were able to be used to identify code inefficiencies.
Christine Cuicchi	CEWES	SPPT	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimization for MPPs' workshop at CEWES MSRC.
Daniel Creighton	CEWES	SPPT	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimiation for MPPs' workshop at CEWES MSRC.
Ross Hall	CEWES	EQM	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimization for MPPs' workshop at CEWES MSRC.
Ross Hall	CEWES	EQM	CRPC/Tennessee	personal contact, workshop	Attended 'Portable Parallel Performance Tools' work-shop at CEWES MSRC.
Rama Valisetty	CEWES	SPPT	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimiation for MPPs' workshop at CEWES MSRC.
Rama Valisetty	CEWES	SPPT	CRPC/Tennessee	personal contact, workshop	Attended 'Portable Parallel Performance Tools' work-shop at CEWES MSRC.
Jerry Ballard	CEWES	EQM	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimiation for MPPs' workshop at CEWES MSRC.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Joe Schmidt	CEWES	SPPT	CRPC/Rice	personal contact	Discuss specifications for programming library to allow separate MPI codes to trade boundary information with each other.
Brian Jean	CEWES	SPPT	CRPC/Rice	personal contact	Discuss specifications for programming library to allow separate MPI codes to trade boundary information with each other.
Alan Stagg	CEWES	SPPT	CRPC/Rice	personal contact	Discuss specifications for programming library to allow separate MPI codes to trade boundary information with each other.
Alan Stagg	CEWES	SPPT	CRPC/Tennessee	personal contact, workshop	Attended ‘Performance Evaluation of Parallel Systems’ workshop at CEWES MSRC.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Mike Cozart Sheile McCollum Mike Scott Randy Chapman Clay Bearden Ricky Burger Karl Kneile Ron Turner Don Atkins Randy Sloan Stephen Powell Rusty Zarclor Donna Pemberton Julie Van Hooser Kenny McDonald Peter Montgomery Shih Chen	AEDC	SPPT	CRPC/Tennessee	personal contact, workshop	Attended ‘Parallel Tools and Libraries’ workshop at AEDC.
Alex Carrillo	CEWES	SPPT	CRPC/Tennessee	pesonal contact, workshop	Attended ‘Portable Parallel Performance Tools’ work-shop at CEWES MSRC.
Alex Carrillo	CEWES	SPPT	CRPC/Tennessee	personal contact, workshop	Attended ‘Performance Eval-uation of Parallel Systems’ workshop at CEWES MSRC.
Alex Carrillo	CEWES	SPPT	CRPC/Tennessee	personal contact, workshop	Attended ‘Parallel Tools and Libraries’ workshop at CEWES MSRC.
Fred Tracy	CEWES	SPPT	CRPC/Rice	personal contact, workshop	Attended ‘Parallel Tools and Libraries’ workshop at CEWES MSRC.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Alan Wallcraft	NRL	CWO	CRPC/Tennessee	e–mail	Jack Dongarra, Clint Whaley, and Antoine Petitet corresponded with Alan Wallcraft about the possiblity of using ScaLAPACK for the ocean modeling challenge problem (June – July 1997).
David Medina	Philips Lab, Kirtland AFB	CFD	CRPC/Rice	personal contact	Consulted on parallelization techniques for MAGI code.
Ted Carney	New Mexico Tech	CFD	CRPC/Rice	phone call, e–mail	Discussion on MAGI code (Ted is an author of the MAGI code).
Doug Strasburg	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimization for MPPs' workshop at CEWES MSRC.
Doug Strasburg	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Rice	visit	To discuss use of parallel tools in code migration. A focused effort on Helix code optimization is proposed for the next year.
Dan Nagle	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Rice	personal contact	Collaborate on code migration projects and creation of CMG in–house tools.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Henry Gabb	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Rice	personal contact	Collaborate on code migration projects, especially Fortran 90 bindings of POSIX threads for MAGI code.
Phil Bording	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Rice	personal contact	Collaborate on code migration projects.
Jay Cliburn	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Rice	personal contact	Collaborate on code migration projects.
James White	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Rice, Tennessee	personal contact, e–mail	Collaborate on installation and testing of TotalView debugger on CEWES MSRC platforms.
Paul Adams	Computationl Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended ‘Code Optimization for MPPs’ workshop at CEWES MSRC.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Phil Bording	Computational Mgiration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimization for MPPs workshop at CEWES MSRC.
Dave Sanders	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended 'Portable Parallel Performance Tools' workshop at CEWES MSRC.
Carol Beaty	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended 'Portable Parallel Performance Tools' workshop at CEWES MSRC.
Carol Beaty	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended 'Code Optimization for MPPs' workshop at CEWES MSRC.
Henry Gabb	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended 'Portable Parallel Performance Tools' workshop at CEWES MSRC.

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Dan Nagle	Computational Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended ‘Performance Evaluation of Parallel Systems’ workshop at CEWES MSRC.
Paul Adams	Computationla Migration Group, CEWES MSRC	Code migration	CRPC/Tennessee	personal contact, workshop	Attended ‘Parallel Tools and Libraries’ workshop at CEWES MSRC.
John Petillo	SAIC	CFD	MSU	BYOC workshop	Training
Henry Freund	SAIC	CFD	MSU	BYOC workshop	Training
Michael Haffel	NRL	N/A	MSU	BYOC workshop	Training
Richard Mowrey	NRL	CCM/CWO	MSU	BYOC workshop	Training
Brett Dunlap	NRL	CCM	MSU	BYOC workshop	Training
Felix Burt	NRL	N/A	MSU	BYOC workshop	Training
Sandy Landsberg	NRL	CFD	MSU	conference	Collaboration
Andy Wissink	MCAT	CFD	MSU	conference	Collaboration
Bob Meakin	NAS	CFD	MSU	conference	Collaboration
William Chan	MCAT	CFD	MSU	conference	Collaboration
John Benek	Microcraft	CFD	MSU	conference	Collaboration
Fernando Grinstein	NRL	CFD	MSU	conference	Collaboration
Frank Caradonna	NAS	CFD	MSU	phone	Collaboration
David Medina	PL/K	CFD/CSM	MSU	outreach visit	Collaboration/Training
Ralph Noack	WRITE	CFD	MSU	phone	Collaboration

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
David Fyfe	NRL	CFD	MSU	phone	Collaboration
Ravi Ramamutri	NRL	CFD/CSM	MSU	phone	Collaboration
Gary Brown	CEWES/CHL	CFD/EQM	MSU	outreach visit	User support
Ross Hall	CEWES/CHL	CFD/EQM	MSU	outreach visit	User support
Bonnie Heikkinen	AEDC	CFD	MSU	phone	Collaboration/training
Bobby Nichols	AEDC	CFD	MSU	phone	Collaboration
Jay Boris	NRL	CFD	MSU	conference	Coordination
Eswar Josyula	ASC	CFD	MSU	conference	User support
Don Davis	Elec. Boat	CFD	MSU	conference	Collaboration
Craig Wagner	Elec. Boat	CFD	MSU	conference	Collaboration
Miguel Visbal	ASC	CFD/EQM	MSU	conference	User support
Susan Polsky	NSWCD	CFD	MSU	conference	User support
Joseph Baum	SAIC	CFD	MSU	conference	User support
Jim Brock	WRITE	CFD	MSU	conference	User support
Leon Chandler	PL/K	CEA	MSU	conference	User support
Charlie Berger	CEWES	CFD	MSU	outreach visit	Collaboration/training
Bob Bernard	CEWES	CFD	MSU	outreach visit	Collaboration/training
Billy Johnson	CEWES	CFD	MSU	outreach visit	Collaboration/training
Norm Scheffner	CEWES	CFD	MSU	outreach visit	Collaboration/training
Richard Stockstill	CEWES	CFD	MSU	outreach visit	Collaboration/training
Rao Vemulakonda	CEWES	CFD	MSU	outreach visit	Collaboration/training
Dave Belk	WRITE	CFD	MSU	phone	User support

CEWES MSRC User	User Site	Technical Area	CEWES MSRC PET Team Member	Mode of Contact	Purpose/Result of Contact
Raju Namburu	CEWES	CSM	NCSA	visit, e–mail	Discuss coupling of CTH and Dyna3D. Project proposed for Year 3
Steve Akers	CEWES	CSM	NCSA	visit, phone call, e–mail	Develop Dyna3D to Epic translator, parallelization of EPIC on SGI Origin2000
Robert Hall	CEWES	CSM	NCSA	visit, phone call, e–mail	Discuss coupling of CTH and Dyna3D. Project proposed for Year 3
Jon Windham	CEWES	CSM	NCSA	visit	Discuss developing material model for CTH (future proposal)
Doug Strasburg	CEWES	CSM	NCSA	visit	Discuss developing material model for CTH (future proposal)
Raju Namburu	CEWES	CSM	CAU	visit	Discussion/status briefing

Table 4
TOOLS IMPLEMENTED

Tool	Status	Purpose	CEWES MSRC Users	Providing Institution(s)	Impact
CFD					
Fortran interface for Pthreads	Being worked on	Develop Fortran 90 bindings for the POSIX threads functions	Any CEWES MSRC code developer or user	MSU ERC CRPC/Rice	An alternative approach for potentially higher performance shared–memory parallel programming
MPE graphics library	Delivered	Real–time, asynchronous drawing to X11 window	Any CEWES MSRC code developer or user	MSU ERC CRPC/Rice Argonne	Able to visualize data during execution of parallel solvers. Aids diagnostics & postprocessing
Unstructured Message–Passing Toolkit	Delivered	Provide users with model data structure and associated functions to simplify the development of scalable message–passing software	Any CEWES MSRC unstructured code developer or user	MSU ERC	Enhanced performance of unstructured CFD solvers
Unstructured Mesh Element Graph Finder	Delivered	Efficient algorithm to determine element connectivity	Any CEWES MSRC unstructured code developer or user	MSU ERC	Enhanced performance of unstructured CFD solvers

Tool	Status	Purpose	CEWES MSRC Users	Providing Institution(s)	Impact
CSM					
Damage Assessment and Residual Capacity Environment	Under development	CAD/INGRID/ DYNA3D interface	R. Namburu	Clark Atlanta	Facilitate damaged structures modeling
Dyna3D to Epic Translator (d2e)	Installed/being worked on	Translate Dyna3D format file to EPIC format files	Steve Akers & others in the CEWES Structures Lab	NCSA	Reduce job preparation time by 25–50%
FMS					
Provider Tango WebWisdom	Installed at CEWES MSRC and JSU	Distance Collaboration and Education	All interested in remote collaboration and training	Syracuse	CSC 499, both taught by Syracuse
Grid Generation Search Engine	Supported at Syracuse	Facilitate discovery of grid generation information	Users in grid–related CTAs (CFD, CSM, CWO, EQM)	Syracuse	Provides higher signal–to–noise ratio in accessing Internet
CEWES MSRC Search Engine	Supported at Syracuse	Provides search capability for CEWES MSRC website	Users of the CEWES MSRC website	Syracuse	Provides search capability for CEWES MSRC website
Website Management System	Under development at Syracuse	Facilitate managment of CEWES MSRC website	Users of the CEWES MSRC website	Syracuse	Facilitate management of large amounts of rapidly changing information

Tool	Status	Purpose	CEWES MSRC Users	Providing Institution(s)	Impact
SPPT					
VAMPIR performance analysis tool	Installed, tested and evaluated on the Cray T3E, IBM SP and SGI Origin 2000 at CEWES MSRC	Document and record statistics of significant events (e.g., subroutine calls, sending or receiving messages, I/O) within the execution of user codes	Any CEWES MSRC code developer	CRPC/Tennessee, Pallas GmbH (Germany)	Assist users in the determination of execution and message–passing patterns in order to further optimize their code; VAMPIR was used to find improvements in the communication performance of the Challenge code ICEPIC from AFRL
MPE logging library and nupshot performance analysis tool	Installed, tested and evaluated on the SGI Power Challenge Array and Origin 2000 at CEWES MSRC; developed new version of nupshot to function under multiple versions of the Tc1 and TK graphics libraries	Document and record statistics of significant events (e.g., subroutine calls, sending or receiving messages, I/O) within the execution of user codes	Any CEWES MSRC code developer	CRPC/Tennessee, Argonne	Assist users in the determination of execution and message–passing patterns in order to further optimize their code
AIMS performance analysis tool	Installed, tested and evaluated on the IBM SP and SGI Power Challenge Array; working with developers to correct bugs found in current release	Document and record statistics of significant events (e.g., subroutine calls, sending or receiving messages, I/O) within the execution of user codes	Any CEWES MSRC code developer	CRPC/Tennessee, NASA Ames NAS Division	Assist users in the determination of execution and message–passing patterns in order to further optimize their code

Tool	Status	Purpose	CEWES MSRC Users	Providing Institution(s)	Impact
SvPablo performance analysis tool	Installed, tested and evaluated on the SGI Power Challenge Array and Origin 2000; working with developers to create more robust version of tool for use at CEWES MSRC	Document and record statistics of significant events (e.g., subroutine calls, sending or receiving messages, I/O), within the execution of user codes	Any CEWES MSRC code developer	CRPC/Tennessee, Pablo group at Illinois	Assist users in the determination of execution and message–passing patterns in order to further optimize their code
ParaDyn interactive performance analysis tool	Installed, tested and evaluated on the IBM SP at CEWES MSRC	Analyze running code for potential bottlenecks, and document and record statistics of significant events (e.g., subroutine calls, sending or receiving messages, I/O) within the execution of user codes	Any CEWES MSRC code developer	CRPC/Tennessee, ParaDyn Group at Wisconsin	Assist users in the determination of execution and message–passing patterns in order to further optimize their code

Tool	Status	Purpose	CEWES MSRC Users	Providing Institution(s)	Impact
TotalView parallel debugger	Unable to install on SGI Power Challenge Array and Origin 2000 at CEWES MSRC due to message–passing library version conflict; installed but unable to run on IBM SP due to batch queue conflicts; user demand for a good cross–platform debugger calls for quick resolution to these problems	Analyze running code for tracking down causes of incorrect computations and catastrophic execution errors	Any CEWES MSRC code developer	CRPC/Tennessee, Dolphin Interconnect Solutions	Assist users in locating fatal errors and other problems within their codes
MPE graphics library	Created Fortran 90 module to draw colored contour plots for two–dimensional, unstructured grids on SGI Origin 2000 at CEWES MSRC; potentially available on any HPC platform with F90, MPI and X Windows	Asynchronously draw color graphics to an X11 window during the course of a numerical simulation	Any CEWES MSRC code developer or user	CRPC/Rice, MSU ERC, Argonne	Able to visualize data as it was being generated by parallel code in order to monitor the accuracy and progress of the solution

Tool	Status	Purpose	CEWES MSRC Users	Providing Institution(s)	Impact
ScaLAPACK	Installed, tested and evaluated on the Cray T3E, IBM SP and SGI Origin 2000 at CEWES MSRC	Library of routines for the solution of dense, band and tridiagonal linear systems of equations and other numerical computations	Any CEWES MSRC code developer	CRPC/Tennessee	Allows users to call library subroutines rather than code complex computations; used in the Wallcraft Ocean Modeling challenge application to achieve a significant improvement in performance
PETSc (Portable, Extensible Toolkit for Scientific Computation)	Installed on IBM SP at CEWES MSRC	Compare relative merits of parallel libraries and languages (HPF)	Application programmers interested in using HPF or PETSc library	CRPC/Rice, Argonne	Evaluation will help users to choose better methods for parallel computations on different parallel platforms
Repository in a Box (RIB)	Installed and tested at CEWES MSRC WWW server	Toolkit for setting up and maintaining software repositories	CEWES MSRC code developers	CRPC/Tennessee	Provides a uniform interface to a software catalog for users to search for codes already written that solve the same or similar problems before attempting to create a completely new code

Tool	Status	Purpose	CEWES MSRC Users	Providing Institution(s)	Impact
MPICH–on–T3E	Being finalized (cleanup and polish)	To provide a high performance port of MPICH that targets the Cray T3E	CEWES MSRC users of the Cray T3E and those who program using MPI	MSU ERC	This project will enable the Cray T3E to be included in the list of MPICH supported platforms. This will allow CEWES MSRC programmers to write portable MPI code that can be used on the T3E as well as the 02K and SP machines that are present at CEWES MSRC.
SV					
VisGen Tool for EQM	First release delivered, development is on–going	Visualization	Cerco, Noel, other EQM/CWO	NCSA	Provides support for cross–platform vis of highly multivariate data
Damaged structures visualization	Demonstrated at SC'97, in use by scientists	Visualization	Namburu, Papados, Bevins, Armstrong, other CSM	NCSA	Supports visual analysis of large–data simulation results
Image– and movie–capture code	Development is on–going	Web–sharing	Potentially all	NCSA	Enables Web–sharing of vis output
The Visualization ToolKit	Package is in place, available for use	Tool development	Potentially all	GE R&D	Provides easy–to–use vis toolkit
NCSA vss 2.2	Development is on–going	Data sonification	Potentially all	NCSA	Provides easy entry into new data analysis technique

Table 5 CEWES MSRC USER CODES IMPACTED				
Code	**Nature of Code**	**CEWES MSRC User**	**Institutions Involved**	**Result**
CFD				
TURB3D	CFD solver	Fernando Grinstein	MSU	Currently working on optimization of scalable version
Parallel MAGI	CFD solver	David Medina	MSU	Currently working on optimization of scalable version
OVERFLOW	3D, time–accurate, compressible, Chimera multi–zone, RANS solver	Bob Meakin	MSU	Ported to T3E
FAST3D	CFD solver	Sandy Landsberg	MSU	Ported to SP
CH3D	3D Hydrodynamics	Billy Johnson	MSU	MPI parallel implementation
HIVEL2D	Shallow–water solver	Charlie Berger	MSU	Added and demonstrated computational design capability
CSM				
DYNA3D	Structural FEM	R. Namburu	CAU	Data conversion and preliminary visualization of DYNA3D models

Code	Nature of Code	CEWES MSRC User	Institutions Involved	Result
CWO				
WAM cycle 4 wind wave model	CWO code	Bob Jensen	Ohio State CEWES MSRC	Added unsteady currents option to WAM; added unsteady depths option to WAM; implemented modified wind input algorithm, to account for the presence of currents; worked with Zhang (OSU) on 2–way coupling of WAM with CH3D marine circulation model
CH3D–s, sequential version of the marine circulation model	CWO code	Billy Johnson	Ohio State CEWES MSRC	Added radiation stress to CH3D–s, added wave stress to CH3D–s, modified the CH3D–s temperature computation code, simulated Kelvin wave propagation in Lake Michigan, developed an interface that interactively 2–way couples the CH3D and WAM models
CH3D–p, parallel version of the marine circulation model	CWO code	Billy Johnson	Ohio Stae CEWES MSRC	Installed model on the CRAY T3E at OSC, deployed CH3D–p in Lake Michigan and achieved stable runs, compared the results of parallel and sequential computations

Code	Nature of Code	CEWES MSRC User	Institutions Involved	Result
CH3D–SED, marine circulation model, with integrated sediment transport sub–model	CWO code	Billy Johnson	Ohio State CEWES MSRC	Deployed CH3D–SED in Lake Michigan, detected technical problems associated with strong undulations of the Lake Michigan bottom topography, modified and verified the CH3D–SED code for the computation of the temperature field, achieved stable CH3D–SED runs on both SGI and Cray platforms
EQM				
CE–QUAL–ICM	EQM water quality model	Mark Dortch Carl Cerco Barry Bunch Mark Noel CEWES Environmental Lab	Texas CEWES	Parallelized for T3E, 02k and SP machines. Currently being used in production mode.
ADCIRC	EQM hydrodynamics model	Norm Scheffner Rao Vemulokanda CEWES Environmental Lab	Texas CEWES	Parallelized for SP and T3E. Currently being tested for various machines and data.
FMS				
Comprehensive Mine Simulator (CMS)	FMS application	Steve Bishop FMS users in general	Army Night Vision Lab Syracuse CEWES NVL	Assess potential and strategy for parallelization of code

Code	Nature of Code	CEWES MSRC User	Institutions Involved	Result
Modular Simulation of Armed Forces (ModSAF)	FMS Application	FMS users in general	Syracuse CEWES	Procured and installed package
SPPT				
MAGI	Smooth particle hydrodynamics (SPH) code	David Medina	Philips Lab Kirtland AFB CRPC/Rice Computational Migration Group	Fortran 90 bindings for POSIX threads were created by Breshears, Gabb and Bova in order to parallelize the MAGI code. Use of pthreads has yielded encouraging results.
Matrix Inverter	Ocean model code boundary condition preprocessor	Alan Wallcraft	NAVO PSC CRPC/Rice Tennessee	Routines from the ScaLAPACK library were successfully used to construct a matrix inversion code for the initial boundary conditions of a global ocean model.
ICEPIC	3D Cartesian PIC code	Jerry Sasser Sheri Colella Larry Merkle	AFRL CRPC/Tennessee	Found inefficient message passing strategies within code using performance analysis tools (VAMPIR). Modifications to portions of the code resulted in a significant speed up.
POSIX Pthreads library	Standardized library for creation, control and termination of multi–threaded code executions	Potentially any CEWES MSRC user	CRPC/Rice MSU ERC CEWES MSRC CMG	Created Fortran 90 binding for POSIX threads standard.

Code	Nature of Code	CEWES MSRC User	Institutions Involved	Result
MPE graphics library	Set of routines that can asynchronously draw color graphics to an X11 window during the course of a numerical simulation	Potentially any CEWES MSRC user	CRPC/Rice MSU ERC Tennessee	Created Fortran 90 module for accessing the routines as well as adding new functionality.
nupshot/MPE logging	Performance analysis tools	Any CEWES MSRC application developer	CRPC/Tennessee	Both tools have been modified to work correctly and robustly on CEWES MSRC platforms. Newer versions of Tck/Tk (later versions of Tc1/Tk run on SGI IRIX 6 platforms, earlier version does not), as well as porting the MPE logging library to vendor MPIs and removing bugs.
AIMS	Performance analysis tool	Any CEWES MSRC application developer	CRPC/Tennessee LANL	Bugs have been found and reported, including failure to instrument the MPI_SendRecv call, incorrect statistical analysis results, and crashes of the instrumentor GUI when large numbers of files are loaded. The Los Alamos tools team is taking on the task of implementing Fortran 90 support for AIMS in direct response to requests from CEWES MSRC users.

Code	Nature of Code	CEWES MSRC User	Institutions Involved	Result
ParaDyn	Performance analysis tool	Any CEWES MSRC application developer	CRPC/Tennessee Wisconsin	University of Tennessee PET team tested the IBM SP MPI version of the Paradyn 2.0 release and reported a bug that was causing Paradyn to crash frequently when used to run and monitor an MPI application with more than twelve processes. UTK tested Paradyn with Fortran programs and reported problems with the Paradyn Fortran interface which have subsequently been fixed. UTK also suggested improvements in the user interface which are being implemented in the next release.
SGI BLAS	Vendor–optimized Basic Linear Algebra Subroutines	Any CEWES MSRC application developer	CRPC/Tennessee SGI/Cray	UTK PET team reported a performance bug in the SGI implementation of one of the BLAS routines, tested the patch from SGI to verify that it fixed the problem, and worked with CEWES MSRC staff to get the patch installed.
Cray T3E MPI	Vendor–supported Message Passing Interface library	Any CEWES MSRC application developer	CRPC/Tennessee SGI/Cray	UTK PET team has reported several bugs in several releases of Cray MPI for the T3E, most of which have been fixed.

Code	Nature of Code	CEWES MSRC User	Institutions Involved	Result
Cray C Compiler	Vendor–supported C language compiler	Any MSRC application developer	CRPC/Tennessee SGI/Cray	UTK reported a bug in the Cray C compiler for the T3E which SGI/Cray has agreed exists and is investigating how to fix.

Table 6
TECHNOLOGY TRANSFER

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
CFD					
Legacy code parallelization expertise		MSU ERC	User training	CEWES CHL	Enhanced simulation capability by making user software available on new CEWES MSRC platforms
The DoD Fortran code MAGI is being used to investigate the feasibility of threads based parallel programming		MSU ERC CRPC/Rice Nichols CMG	Demonstration of alternative means to optimize shared memory parallelism	Phillips Lab, Kirtland AFB	More scalable and efficient parallel software
Introduction and demonstration of computational design		MSU ERC	User training and demonstration of advanced CFD technology	CEWES CHL	Introduction of a new design tool applicable to high velocity flood control channels

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
EQM					
Space–filling curve algorithm	Texas	Texas	Partitioning of finite element meshes for parallel processing	Carl Cerco Mark Noel	Allows for load balancing and parallel scalability of codes
Perl script for web–based code launching	Texas	Texas	To demonstrate capability of launching a parallel code from a website	Jeff Holland (potential)	Could allow for web–based launching of simulators within the Groundwater Modeling System and Surface Water Modeling System
WQMPP, Water Quality Model Pre and Post Processor	Texas	Texas	To read global mesh and data input files and partition them for parallel processing	Carl Cerco Mark Noel	Allowed for a scalable parallelization of CE–QUAL–ICM
SPPT					
Designing and Building Parallel Programs	Ian Foster	CRPC/Rice	An organized, general approach to parallel programming used in several CEWES MSRC training courses	Tutorial attendees	Better use of programmer time in migrating research codes
MPE Graphics Library	MPICH distribution from Argonne/MSU	CRPC/Tennessee	Allows parallel processes in MPI program to write to common X display	CEWES MSRC users who program using MPI	Allows real–time data visualization from simulations using common graphics routines

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
ScaLAPACK	Tennessee	CRPC/Tennessee	Portable, efficient, scalable, easy–to–use library of commonly used dense linear algebra routines	Alan Wallcraft	Significant improvement in application performance
VAMPIR	Pallas	CRPC/Tennessee	Performance visualization and analysis of MPI and HPF parallel programs	Jerry Sasser, Kirtland AFB	Significant improvement in communication performance of challenge application code (ICEPIC)
AIMS	NASA Ames NAS Division	CRPC/Tennessee	Performance and visualization and analysis of MPI and PVM message passing programs	All CTAs	Easy–to–use interface with source–code clickback will allow users to quickly spot performance problems and see what parts of their code are causing them.
nupshot	MPICH distribution from Argonne/MSU	CRPC/Tennessee	Performance visualization of MPI parallel programs	All CTAs	Simple easy–to–use tool allows users to get quick view of message–passing behavior of their applications
TotalView	Dolphin Interconnect Systems	CRPC/Tennessee	Debugger for parallel programs	Potential: all CTAs	Excellent parallel debugger highly recommended by other HPC sites that use it

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
Repository in a Box (RIB)	Tennessee	CRPC/Tennessee	Toolkit for setting up and maintaining a software repository, provides uniform interface and inter-operability with other repositories, as well as user discussion forums	Potential: CFD, grid generation, EQM	Promote intra– and inter–CTA sharing of software, algorithms, and experiences
High Performance Fortran (HPF)	High Performance Fortran Forum	CRPC/Rice	Provides high–level data parallelism for Fortran codes	CMG investigating use in MAGI code; interest in principle from Bob Bernard for MAC3D	Much–reduced devel-opment time for migration of ap-propriate codes to parallel platforms
PGHPF	Portland Group, Inc.	CRPC/Rice	An implementation of HPF	CMG	Needed to make use of HPF
High Performance Debugger (HPD)	High Performance Debugger Forum, PTOOLS consortium	CRPC/Rice, Tennessee	Provide a standard-ized debugger for ex-plicitly parallel codes; specification of debugger is in the late draft stage, and implementation ef-forts underway	Potential: any MPI or OpenMP developer	Reduces training time on system when moving to a new ma-chine

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
MPICH–on–T3E	MSU ERC	MSU ERC	Provide a high performance port of MPICH that targets the Cray T3E	CEWES MSRC users of the Cray T3E and those who program using MPI	This project will enable the Cray T3E to be included in the list of MPICH supported platforms. This will allow CEWES MSRC programmers to write portable MPI code that can be used on the T3E as well as the 02K and machines that are present at CEWES MSRC.
C/C					
Web page authoring tools recommendation		NCSA	To provide a list of recommended web authoring tools to aid in the development of CEWES MSRC PET web pages	CEWES MSRC PET web page authors (e.g. CTA leads, PET webmasters)	The impact of the recommendation provided in February 1998 has not yet been realized. A seminar to CTA leads is planned in Year 3 to further technology transfer

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
netWorkPlace	NCSA	NCSA	Promote virtual teams by supplying centralized site for sharing discussions and documents	CEWES MSRC PET team members	netWorkPlace provided a successful site and interface for maintaining the Web–a–Con weekly status report and some discussion. By submitting these reports in one location, they were immediately accessible by all, and provided a space for feedback or additional comments and discussion

Table 7
TRAINING COURSES

Course Title	Location	Duration	Providing Institution	Instructor(s)	Format	No. of Attendees (on–site MSRC users, off–site MSRC users, PET/Integrator Personnel, HBCU/MI personnel, Other)	Overall Rating (out of 5.0)
Parallel Tools & Libraries	AEDC	4/10–4/11/97	CRPC/Tennessee	Christian Halloy	Lecture & labs	18 (16,1,1,0,0)	3.7
Message Passing Interface (MPI)	NRL	5/28–5/30/97	Mississippi State	Puri Bangalore Shane Hebert	Lecture & labs	9 (9,0,0,0,0)	4.4
Parallel Tools & Libraries	CEWES MSRC	7/8–7/9/97	CPRC/Tennessee	Susan Blackford	Lecture & labs, Mbone	10 (2,0,8,0,0)	4.2
Performance Evaluation of Parallel Systems	CEWES MSRC	7/10–7/11/97	CRPC/Tennessee	Erich Strohmaier	Lecture & labs, Mbone	7(2,0,5,0,0)	4.0
CRAY T3E Applications Programming	CEWES MSRC	7/15–7/18/97	SGI/Cray	Kim Snyder	Lecture & labs	7 (3,0,3,1,0)	4.0
Java & the World Wide Web	CEWES MSRC	7/23–7/25/97	Syracuse	Nancy McCracken	Lecture & labs, Web–based	10 (3,0,1,6,0)	4.5
Message Passing Interface (MPI)	NRL	7/28–7/30/97	Mississippi State	Puri Bangalore Shane Hebert	Lecture & labs	17 (11,6,0,0,0)	4.3
IBM SP Programming	CEWES MSRC	7/30–7/31/97	OSC	Armen Ezekielian	Lecture, Mbone	8 (3,0,5,0,0)	4.6

Course Title	Location	Duration	Providing Institution	Instructur(s)	Format	**No. of Attendees** (on–site MSRC users, off–site MSRC users, PET/integrator Personnel, HBCU/MI personnel, Other)	Rating
Visualization Systems & Toolkits	CEWES MSRC	8/26–8/27/97	NCSA	Jay Jackson	Lecture	6 (1,1,3,1,0)	3.7
C++ Programming	CEWES MSRC	9/23–9/25/97	OSC	David Ennis	Lecture & labs, Mbone	20 (3,15,2,0,0)	4.3
SGI ProDev Workshop	CEWES MSRC	10/6–10/10/97	SGI/Cray	Robert Cromartie	Lecture & labs	5 (0,0,5,0,0)	4.3
Message Passing Interface (MPI)	NRL	10/22–10/24/97	Mississippi State	Tony Skjellum Shane Hebert	Lecture & labs	16 (13,3,0,0,0)	4.0
Message Passing Interface (MPI)	CEWES MSRC	10/29–10/31/97	Mississippi State	Puri Bangalore Shane Hebert	Lecture & labs	10 (2,1,7,0,0)	4.4
Parallel Programming Workshop for Fortran Programmers	NRL	11/4–11/6/97	NRC, Mississippi State	Dan Nagle Steve Bova	Hands–on labs	6 (5,1,0,0,0)	4.8
CTH: A Software Family for Multi-dimensional Continuum Mechanics Analysis	CEWES MSRC	12/17–12/19/97	Sandia	Gene Hertel	Lecture & labs	12 (8,2,2,0,0)	4.5
Techniques in Code Parallelization	CEWES MSRC	1/15–1/16/98	Texas	Mary Wheeler Carter Edwards Victor Parr Clint Dawson Monica Martinez	Lecture	19 (10,2,7,0,0)	4.0

Course Title	Location	Duration	Providing Institution	Instructur(s)	Format	**No. of Attendees** (on–site MSRC users, off–site MSRC users, PET/integrator Personnel, HBCU/MI personnel, Other)	Rating
Portable Parallel Performance Tools	CEWES MSRC	1/27–1/28/98	CRPC/Tennessee	Shirley Browne Clay Breshears	Lecture & labs, Mbone	8 (3,0,5,0,0)	4.0
Code Optimization for MPPs	CEWES MSRC	2/4–2/6/98	CRPC/Tennessee	Phil Mucci Kevin London	Lecture & labs, Mbone	12 (5,0,6,0,1)	4.3
Parallel Programming Workshop for Fortran Programmers	AEDC	3/3–3/6/98	NRC, Mississippi State	Dan Nagle Rick Weed	Hands–on labs	8 (7,1,0,0,0)	5.0
Parallel Programming for Fortran Programmers	NRL	3/17–3/20/98	NRC, CRPC/Rice	Dan Nagle Clay Breshears	Hands–on labs	3 (2,1,0,0,0)	4.5

Table 8
TRAINING COURSES & SEMINARS at HBCU/MIs

Course Title	**Location**	**Duration**	**Providing Institution**	**Instructor(s)**	**Format**	**Number of Attendees** Undergraduates Graduate Students Faculty/Staff
1997 Introductory HPC Summer Institute	JSU	5/27–6/6/97	JSU	David Pratt	Morning lectures, Afternoon lab exercises	15 undergraduate students
CSC 499–01 Programming for the Web	JSU	Fall 1997 Semester	JSU Syracuse	Geoffrey Fox Nancy McCracken Tom Scavo Debasis Mitra	Web–based distance learning class	14 undgraduate students
CSC 499–01 Programming for the Web	JSU	Fall 1997 Semester	JSU Syracuse	Geoffrey Fox Nancy McCracken Tom Scavo Debasis Mitra Qutaibah Malluhi	Web–based distance learning class	7 undergraduate students 2 graduate students (auditing the class)
PVMPI	JSU	1 hour, October 30	CRPC/Tennessee	Graham Fagg	Seminar	31 faculty, staff, & students
High Performance Computing Application & Technology (HiPCAT)	CAU	3/5–3/6/98	CAU CEWES MSRC PET Team Members	N/A	Symposium	100+
ISI	CAU	2 weeks	CAU	B. Bryan S. Sarathy O.Olatidoye	Workshop	15

Table 9
HBCU/MI STUDENTS IMPACTED

Introductory High Performance Computing Summer Institute May 27 – June 6, 1997			
Student	**Level**	**Major**	**University**
Sherry L. Caldwell	Sophomore	Math/Computer Science	Tougaloo College
Stefen L. King	Sophomore	Math/Physics	Tougaloo College
Catina Folsom	Senior	Computer Science/Business Administration	Rust College
Cassandra T. Lesueur	Junior	Computer Science/Business Administration	Rust College
Taheerah Fulgham	Sophomore	Computer Science	Jackson State University
Nikita P. Magee	Sophomore	Computer Science/Applied Math	Alcorn State Univesity
Wayne Jackson	Junior	Computer Science	Jackson State University
Kimberly M. Neal	Junior	Computer Science	Jackson State University
Heather M. Johnson	Sophomore	Computer Science	Rust College
Robert L. Stewart	Sophomore	Computer Science	Jackson State University
Kenya T. Johnson	Sophomore	Computer Science	Alcorn State University
Cedric A. Terry	Junior	Computer Science/Math	Jackson State University
Denetrice King	Junior	Computer Science/Applied Math	Alcorn State University
Timothy J. Ward	Junior	Computer Science	Jackson State University
Kendrick Wilson	Sophomore	Computer Science	Jackson State University

CSC–499 WEB Programming Fall, 1997			
Student	**Level**	**Major**	**University**
Hilda L. Alexander	Senior	Computer Science	Jackson State University
Camarian Bays	Senior	Computer Science	Jackson State University
Donald Crayton	Junior	Computer Science	Jackson State University
Richard Hall	Junior	Computer Science	Jackson State University
Chastidy S. Harris	Junior	Computer Science	Jackson State University
Tiffany Hughes	Senior	Computer Science	Jackson State University
Jocelyn Coleman	Junior	Computer Science	Jackson State University
Mishi C. Jones	Junior	Computer Science	Jackson State University
Nicklaus McKnight	Senior	Computer Science	Jackson State University
Naquisha L. Smith	Senior	Computer Science	Jackson State University
Cedric Terry	Senior	Computer Science	Jackson State University
Timothy Ward	Junior	Computer Science	Jackson State University
Jamie Williams	Junior	Computer Science	Jackson State University
Alex J. Wilson	Junior	Computer Science	Jackson State University

CSC–499 WEB Programming Spring, 1998			
Student	**Level**	**Major**	**University**
Krystal Cooper	Freshman	Computer Science	Jackson State University
Gloria A. Davenport	Senior	Computer Science	Jackson State University
Douglas W. Holton	Senior	Computer Science	Jackson State University
Mitchell D. Lee	Senior	Computer Science	Jackson State University
Angela A. Robinson	Senior	Computer Science	Jackson State University
Dionte S. Wilson	Senior	Computer Science	Jackson State University
Marvin A. Winfield	Senior	Computer Science	Jackson State University

Students at Clark Atlanta in Undergraduate Research			
Student	**Level**	**Major**	**University**
G. Jones	Undergraduate	Chemical/Civil Engineering	Clark Atlanta University
L. Milligan	Undergraduate	Mechanical Engineering	Clark Atlanta University
C. McIntyre	Undergraduate	Math	Clark Atlanta University